=> d	his	
	(FILE	"HOME' ENTERED AT 14:16:45 ON 17 MAY 2011}
L1	FILE	'CAPLUS' ENTERED AT 14:16:57 ON 17 MAY 2011 1 S US20070015746/PN SELECT RN L1 1-
L2 L3 L4 L5 L6	FILE	'REGISTRY' ENTERED AT 14:17:39 ON 17 MAY 2011 47 S E1-47 10 S L2 AND 5-6-7/SZ 37 S L2 NOT L3 12 S L4 AND 5-7/SZ 25 S L4 NOT L5
L7	FILE	'CAPLUS' ENTERED AT 14:21:12 ON 17 MAY 2011 5 S L5
L8 L9 L10 L11 L12 L13 L14	FILE	"NECISTRY' ENTERED AT 14:23:26 ON 17 MAY 2011 STRUCTURE UPLOADED 50 S L6 3347 S L6 SSS FUL 32 S L10 AND 5-77-SZ STRUCTURE UPLOADED 2040 S L12 SUB-L10 FUL 1307 S L10 NOT L13
L15	FILE	'CAPLUS' ENTERED AT 14:34:30 ON 17 MAY 2011 62 S L14
L16 L17	FILE	'REGISTRY' ENTERED AT 14:35:09 ON 17 MAY 2011 1 S 35165-04-9/RN 1306 S L14 NOT L16
L18	FILE	'CAPLUS' ENTERED AT 14:35:26 ON 17 MAY 2011 59 S L17
L19 L20	FILE	'REGISTRY' ENTERED AT 14:35:51 ON 17 MAY 2011 1 S 57046-64-7/RN 1305 S L17 NOT L19
L21 L22	FILE	'CAPLUS' ENTERED AT 14:36:09 ON 17 MAY 2011 58 S L20 ANALYZE L21 1- RN HIT : 1266 TERMS
L23 L24 L25	FILE	'REGISTRY' ENTERED AT 14:36:29 ON 17 MAY 2011 1 S 629664-81-9/RN 1182 S 236.13.8/RID 123 S L20 NOT L24
L26	FILE	'CAPLUS' ENTERED AT 14:37:34 ON 17 MAY 2011 39 S L25
L27 L28	FILE	'REGISTRY' ENTERED AT 14:38:11 ON 17 MAY 2011 107 S L25 AND CAPLUS/LC 16 S L25 NOT L27

=> d 18 L8 HAS NO ANSWERS L8 STR

G1:C,N G2:O,S,N

Structure attributes must be viewed using STN Express query preparation.

-> d 112 L12 HAS NO ANSWERS L12 STR



G1:C,N G2:O,S,N

Structure attributes must be viewed using STN Express query preparation.

-> d 128 16

L28 ANSWER 16 OF 16 REGISTRY COPYRIGHT 2011 ACS on STN

RN 1139-56-6 REGISTRY

Entered STN: 16 Nov 1984

ED CN Furo[2,3-d]pyrrolo[3,2,1-jk][1]benzazepine (8CI, 9CI) (CA INDEX NAME)

MF C14 H9 N O CI RPS

L28 ANSWER 15 OF 16 REGISTRY COPYRIGHT 2011 ACS on STN

RN 7486-12-6 REGISTRY

ED Entered STN: 16 Nov 1984

CN Pyrrolo[3',4':3,4]cyclobut[1,2-d]imidazole (8CI, 9CI) (CA INDEX NAME)

MF C7 H3 N3 CI RPS



L28 ANSWER 14 OF 16 REGISTRY COPYRIGHT 2011 ACS on STN

RN 80294-50-4 REGISTRY

ED Entered STN: 16 Nov 1984

CN Oxazolo[5,4-d][1,4]thiazino[2,3,4-jk][1]benzazepine (9CI) (CA INDEX NAME)

MF C13 H8 N2 O S CI RPS

L28 ANSWER 13 OF 16 REGISTRY COPYRIGHT 2011 ACS on STN

RN 80294-51-5 REGISTRY

ED Entered STN: 16 Nov 1984

CN [1,4]Thiazino[2,3,4-jk]thiazolo[5,4-d][1]benzazepine (9CI) (CA INDEX

NAME) MF C13 H8 N2 S2

CI RPS

L28 ANSWER 12 OF 16 REGISTRY COPYRIGHT 2011 ACS on STN

RN 87208-25-1 REGISTRY

RN 87208-25-1 REGISTRY ED Entered STN: 16 Nov 1984

CN 4,9-Methano-4H-pyrrolo[1,2-a]thieno[3,2-d]azepine (9CI) (CA INDEX NAME)

MF C12 H9 N S CI RPS

$$\bigcirc N \bigcirc S$$

L28 ANSWER 11 OF 16 REGISTRY COPYRIGHT 2011 ACS on STN

RN 88084-57-5 REGISTRY

ED Entered STN: 16 Nov 1984

CN Azirino[2,3,1-hi]thiazolo[5,4-e]indole (9CI) (CA INDEX NAME)

MF C9 H4 N2 S CI RPS

L28 ANSWER 10 OF 16 REGISTRY COPYRIGHT 2011 ACS on STN

RN 93281-43-7 REGISTRY

ED Entered STN: 18 Dec 1984

CN 1H-[1]Benzothieno[5,6-b]azirine (9CI) (CA INDEX NAME)

MF C8 H5 N S CI RPS

L28 ANSWER 9 OF 16 REGISTRY COPYRIGHT 2011 ACS on STN

RN 93281-55-1 REGISTRY

ED Entered STN: 18 Dec 1984

CN 2,6-Methano-1H-[1]benzothieno[5,6-b]azirine (9CI) (CA INDEX NAME)

MF C9 H5 N S CI RPS

L28 ANSWER 8 OF 16 REGISTRY COPYRIGHT 2011 ACS on STN

RN 146340-64-9 REGISTRY

ED Entered STN: 09 Mar 1993 CN 4,7:14,17-Difmino-2,22-metheno-9,12-mitriloazepino[4,3-blazacvclonoadecine (9CI) (CA INDEX NAME)

MF C23 H15 N5

CI RPS SR CA Index Guide or Ring Systems Handbook



L28 ANSWER 7 OF 16 REGISTRY COPYRIGHT 2011 ACS on STN

RN 147184-23-4 REGISTRY

ED Entered STN: 23 Apr 1993 CN 10H-Imidazo[],2-a]thieno[3,2-d]azepine,

CN 1UH-Imidazo[],Z-a]thieno[3,Z-d]azepine, 1U-[1-[2-(4-methoxyphenyl)ethyl]-4-piperidinylidenel- (CA INDEX NAME)

MF C24 H25 N3 O S

CI COM

L28 ANSWER 6 OF 16 REGISTRY COPYRIGHT 2011 ACS on STN

RN 147210-28-4 REGISTRY

ED Entered STN: 27 Apr 1993

CN 5H-Thiazolo[3,2-a]pyrimidin-5-one,

6-[2-[4-(10H-imidazo[1,2-a]thieno[3,2-d]azepin-10-ylidene)-1-

piperidinyl]ethyl]=7-methyl= (CA INDEX NAME)
OTHER CA INDEX NAMES:

CN 10H-Imidazo[1,2-a]thieno[3,2-d]azepine, 5H-thiazolo[3,2-a]pyrimidin-5-one

MF C24 H23 N5 O S2

CI COM

L28 ANSWER 5 OF 16 REGISTRY COPYRIGHT 2011 ACS on STN

RN 188965-71-1 REGISTRY ED Entered STN: 13 May 1997

CN 4H-Pyrrolo[1,2-a]thieno[3,2-d]azepine (9CI) (CA INDEX NAME) C11 H9 N S

MF CI RPS

SR CA Index Guide or Ring Systems Handbook

L28 ANSWER 4 OF 16 REGISTRY COPYRIGHT 2011 ACS on STN

RN 264151-37-3 REGISTRY

ED Entered STN: 09 May 2000 CN 4,9-imino-IH-maphtho[2',3':3,4]cyclobuta[1,2-d][1,2,3]triazole (9CI) (CA INOEX NAME)

MF C12 H6 N4

CI RPS

SR CA Index Guide or Ring Systems Handbook

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L28 ANSWER 3 OF 16 REGISTRY COPYRIGHT 2011 ACS on STN
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RN 279253-81-5 REGISTRY

ED Entered STN: 21 Jul 2000

CN Spiro(cyclohexane-1,10'-[10H]imidazo[1,2-a]thieno[3,2-d]azepine] (9CI) (CA INDEX NAME)

MF C15 H16 N2 S

CI COM, RPS SR CA

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

L28 ANSWER 2 OF 16 REGISTRY COPYRIGHT 2011 ACS on STN

RN 719305-66-5 REGISTRY

ED Entered STN: 30 Jul 2004

CN 4H-Imidazo[1,2-a]oxazolo[4,5-d]azepine (9CI) (CA INDEX NAME) C9 H7 N3 O

MF CI RPS

SR CA Index Guide or Ring Systems Handbook

L28 ANSWER 1 OF 16 REGISTRY COPYRIGHT 2011 ACS on STN

RN 1201795-44-9 REGISTRY ED Entered STN: 11 Jan 2010 CN 4H-Thieno[3',2':4,5]szepino[1,2-a]benzimidazole (CA INDEX NAME)

MF C14 H10 N2 S CI RPS

SR CA Index Guide or Ring Systems Handbook



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=> => d his
     (FILE 'HOME' ENTERED AT 14:16:45 ON 17 MAY 2011)
     FILE 'CAPLUS' ENTERED AT 14:16:57 ON 17 MAY 2011
              1 S US20070015746/PN
                SELECT RN L1 1-
     FILE 'REGISTRY' ENTERED AT 14:17:39 ON 17 MAY 2011
             47 S E1-47
             10 S L2 AND 5-6-7/SZ
L4
             37 S L2 NOT L3
L5
             12 S L4 AND 5-7/SZ
_{\rm L6}
             25 S L4 NOT L5
     FILE 'CAPLUS' ENTERED AT 14:21:12 ON 17 MAY 2011
             5 S L5
     FILE 'REGISTRY' ENTERED AT 14:23:26 ON 17 MAY 2011
L8
               STRUCTURE UPLOADED
             50 S L8
L.9
T-10
           3347 S L8 SSS FUL
             32 S L10 AND 5-7/SZ
L12
               STRUCTURE UPLOADED
           2040 S L12 SUB-L10 FUL
L14
           1307 S L10 NOT L13
     FILE 'CAPLUS' ENTERED AT 14:34:30 ON 17 MAY 2011
             62 S L14
     FILE 'REGISTRY' ENTERED AT 14:35:09 ON 17 MAY 2011
             1 S 35165-04-9/RN
L16
           1306 S L14 NOT L16
     FILE 'CAPLUS' ENTERED AT 14:35:26 ON 17 MAY 2011
L18
             59 S L17
     FILE 'REGISTRY' ENTERED AT 14:35:51 ON 17 MAY 2011
L19
             1 S 57046-64-7/RN
L20
          1305 S L17 NOT L19
     FILE 'CAPLUS' ENTERED AT 14:36:09 ON 17 MAY 2011
             58 S L20
            ANALYZE L21 1- RN HIT : 1266 TERMS
     FILE 'REGISTRY' ENTERED AT 14:36:29 ON 17 MAY 2011
L23
             1 S 629664-81-9/RN
L24
           1182 S 2436.13.8/RID
            123 S L20 NOT L24
     FILE 'CAPLUS' ENTERED AT 14:37:34 ON 17 MAY 2011
L26
             39 S L25
     FILE 'REGISTRY' ENTERED AT 14:38:11 ON 17 MAY 2011
            107 S L25 AND CAPLUS/LC
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16 S L25 NOT L27

FILE 'CAPLUS' ENTERED AT 14:40:10 ON 17 MAY 2011

27 S L26 NOT (2011/SO OR 2010/SO OR 2009/SO OR 2008/SO OR 2007/SO

-> d ibib abs hitstr total

L29 ANSWER 1 OF 27 CAPLUS COPYRIGHT 2011 ACS on STN

ACCESSION NUMBER: 2009:1050008 CAPLUS

DOCUMENT NUMBER: 151:236777
TITLE: FXR agonists for treating vitamin D associated

diseases INVENTOR(S): Harnish, Douglas

PATENT ASSIGNEE(S): Wyeth, John, and Brother Ltd., USA

SOURCE: U.S. Pat. Appl. Publ., 53pp.
CODEN: USXXCO

DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC NUM COUNT: 1

PATENT INFORMATION:

 PATENT NO.
 KIND
 DATE
 APPLICATION NO.
 DATE

 US 20090215748
 A1
 20090827
 US 2006-318039
 20081219

 PRIORITY APPLIA. INFO::
 B
 2007-8307P
 P
 20071220

 ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LISUS DISPLAY FORMAT
 AVAILABLE IN LISUS DISPLAY FORMAT
 AVAILABLE IN LISUS DISPLAY FORMAT

AB Provided are cortain methods of treating at least one condition that can be treated by elevating the vitamin D receptor (USB) activity level in a percent of the provided are cortain methods of modulating levels of Cytochrome P 450, family 27, subfamily B, polypeptide I (CTFZPB) and la 25-dihydroxyvitamin D3 in cells, certain methods of modulating extraorliminations of the contract of the cortain methods of modulating extraorliminations are the contract of the cortain provided provided provided provided (MSB) and the cortain provided (MSB) and the co

parathyroid hormone, serum creatining serum albumin, proteinuria, lipid metabolism, renal lipid deposition, menangial exprasion, glosculocalerosis, kidney inflammation, blood pressure, bone recomption, and bone formation, certain methods of identifying FZE modalators, certain methods of identifications in the control of the control of the control of the certain period of the cer

diagnosing the risk that a patient will develop at least one condition that can be treated by elevating the VDR activity level, and certain methods of characterizing the levels of FZR activity in mammals.

17 629664-83-1 837429-85-3 837429-86-4 837429-88-6 837429-80-0

6-(3,4-Difluoro-benzoyl)-4,4-dimethyl-5,6-dihydro-4H-thieno[2,3-d]azepine-8-carboxylic acid ethyl ester 837429-91-3 837429-92-2 837429-93-3 847865-38-7 847865-98-8 847865-40-1 1088713-88-5

RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(FXR agonists for treating vitamin D associated diseases) 629664-83-1 CAPLUS

RN 629664-83-1 CAPLUS
CN Spiro[azepino[4,5-b]indole-1(2B),1'-cyclopentane]-5-carboxylic acid,
3-(3,4-difluorobenzoyl)-3,6-dihydro-, ethyl ester (CA INDEX NAME)

837429-85-3 CAPLUS CN

Imidazo[4,5-d]azepine-4-carboxylic acid, 6-(4-fluorobenzoyl)-3,6,7,8-tetrahydro-, ethyl ester (CA INDEX NAME)

837429-86-4 CAPLUS

CN 4H-Thieno[2,3-d]azepine-8-carboxylic acid, 6-(3,4-difluorobenzovl)-5,6-dihydro-, ethyl ester (CA INDEX NAME)

837429-88-6 CAPLUS RN CN

Azepino[4.5-b]indole-5-carboxylic acid. 3-(4-fluorobenzoyl)-1,2,3,6,7,8,9,10-octahydro-, ethyl ester (CA INDEX NAME)

N 837429-90-0 CAPLUS

CN 4H-Thieno[2,3-d]azepine-8-carboxylic acid, 6-(3,4-difluorobenzoyl)-5,6-dihydro-4,4-dimethyl-, ethyl ester (CA INDEX NAME)

RN 837429-91-1 CAPLUS

CN Pyrrolo[2,3-d]azepine-2,8-dicarboxylic acid, 6-(3,4-difluorobenzoyl)-1,4,5,6-tetrahydro-4,4-dimethyl-, 2,8-diethyl ester (CA INDEX NAME)

RN 837429-92-2 CAPLUS CN Pyrrolo[2,3-d]azeni

Pyrrolo[2,3-d]azepine-2,8-dicarboxylic acid, 6-(3,4-difluorobenzoyl)-1,4,5,6-tetrahydro-4,4-dimethyl-, 2-ethyl 8-(1-methylethyl) ester (CA INDEX NAME)

RN 837429-93-3 CAPLUS CN Pyrrolo[2,3-d]azenia

Pyrrolo[2,3-d]azepine-2,8-dicarboxylic acid, 6-(3,4-difluorobenzoyl)-1,4,5,6-tetrahydro-1,4,4-trimethyl-, 2-ethyl 8-(1-methylethyl) ester (CA INDEX NAME)

RN 847865-38-7 CAPLUS

CN Spiro[azepino[4,5-b]indole-1(2H),1'-cyclobutane]-5-carboxylic acid, 3-(3,4-difluorobenzoyl)-3,6-dihydro-, ethyl ester (CA INDEX NAME)

RN 847865-39-8 CAPLUS

CN Spiro[azepino 4,5-b]indole-1(2H),1'-cyclopropane]-5-carboxylic acid, 3-(3,4-difluorobenzoyl)-3,6-dihydro-, ethyl ester (CA INDEX NAME)

RN 847865-40-1 CAPLUS
CN Spiro[azepino[4,5-b]indole-1(2H),1'-cyclopropane]-5-carboxylic acid,
3-(3,4-df[luorobenzoyl)-3,6-dihydro-, 1-methylethyl ester (CA INDEX NAME)

RN 1088713-88-5 CAPLUS CN Pyrrolo[2,3-d]azepine-2,8-dicarboxylic acid,

6-(3,4-difluorobenzoyl)-1,4,5,6-tetrahydro-4,4-dimethyl-, 2,8-dimethyl ester (CA INDEX NAME)

OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD (1 CITINGS)

L29 ANSWER 2 OF 27 CAPLUS COPYRIGHT 2011 ACS on STN

ACCESSION NUMBER: 2009:769550 CAPLUS DOCUMENT NUMBER: 151:94051

TITLE: Farnesoid X receptor (FXR) agonists for the treatment of nonalcoholic fatty liver and cholesterol gallstone

INVENTOR(S): Zhang, Songwen; Harnish, Douglas; Evans, Mark J.;

Wang, Juan

PATENT ASSIGNEE(S): Wyeth, John, and Brother Ltd., USA SOURCE: U.S. Pat. Appl. Publ., 61pp. CODEN. HEXYCO

DOCUMENT TYPE: Patent LANGUAGE: English FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO. KIND DATE APPLICATION NO. DATE

US 20090163474 A1 20090625 US 2008-253010 20081016

PRIORITY APPLN. INFO.:

PRIORITY APPLN. INFO.:

US 2008-253010 20081016

16 The invention provides methods for treating nonalcoholic fatty liver disease with farmsoid X receptor (FGS) aponists. The invention also inc [KC], alanine aminotransferase (ALT), aspartate aminotransferase (AST), cytokeratin 18 (CX-18), matrix metalloproteinase-0 (MGT-9), matrix metalloproteinase-0 (MGT-9), matrix metalloproteinase-0 (MGT-14), tissue inhibitor of metalloproteinase of the model of the matrix metalloproteinase of the model of the model

gallstone disease. T 629664-83-1 837429-85-3 837429-86-4 837429-89-7 837429-90-0 837429-91-1

837429-92-2 837429-93-3 847865-38-7 847865-39-8 847865-40-1 1088713-88-5

RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses) (FXR agonist for treatment of nonalcoholic fatty liver and cholesterol

gallstone disease)
RN 629664-83-1 CAPLUS
CN Spiro[azepino[4,5-b]indole-1(2H),1'-cyclopentane]-5-carboxylic acid,

Spiro[azepino[4,5-b]indole-1(2H),1'-cyclopentane]-5-carboxylic acid 3-(3,4-difluorobenzoyl)-3,6-dihydro-, ethyl ester (CA INDEX NAME)

RN 837429-85-3 CAPLUS

N Imidazo[4,5-d]azepine-4-carboxylic acid,

6-(4-fluorobenzoyl)-3,6,7,8-tetrahydro-, ethyl ester (CA INDEX NAME)

RN 837429-86-4 CAPLUS CN 4H-Thieno[2,3-d]azer

4H-Thieno[2,3-d]azepine-8-carboxylic acid, 6-(3,4-difluorobenzoyl)-5,6-dihydro-, ethyl ester (CA INDEX NAME)

RN 837429-89-7 CAPLUS

CN Azepino[4,5-b]indole-5-carboxylic acid, 3-(4-fluorobenzoyl)-1,2,3,6,7,8,9,10-octahydro-1,1-dimethyl-, ethyl ester (CA INDEX NAME)

RN 837429-90-0 CAPLUS

CN 4H-Thieno[2,3-d]azepine-8-carboxylic acid, 6-(3,4-difluorobenzoyl)-5,6-dihydro-4,4-dimethyl-, ethyl ester (CA INDEX NAME)

RN 837429-91-1 CAPLUS CN Pyrrolo[2,3-d]azenia

N Pyrrolo[2,3-d]azepine-2,8-dicarboxylic acid, 6-(3,4-difluorobenzoyl)-1,4,5,6-tetrahydro-4,4-dimethyl-, 2,8-diethyl ester (CA INDEX NAME)

RN 837429-92-2 CAPLUS

CN Pyrrolo[2,3-d]azepine-2,8-dicarboxylic acid, 6-(3,4-difluorobenzyl)-1,4,5,6-tetrahydro-4,4-dimethyl-, 2-ethyl 8-(1-methyl-ethyl) ester (CA INDEX NAME)

RN 837429-93-3 CAPLUS

CN Pyrrolo[2,3-d]azepine-2,8-dicarboxylic acid,
6-(3,4-difluorobenzoyl)-1,4,5,6-tetrahydro-1,4,4-trimethyl-,2-ethyl
8-(1-methylethyl) ester (CA INDEX NAME)

847865-38-7 CAPLUS CN

Spiro[azepino[4,5-b]indole-1(2H),1*-cyclobutane]-5-carboxylic acid, 3-(3,4-difluorobenzoy1)-3,6-dihydro-, ethyl ester (CA INDEX NAME)

RN 847865-39-8 CAPLUS

CN Spiro[azepino[4,5-b]indole-1(2H),1'-cyclopropane]-5-carboxylic acid, 3-(3,4-difluorobenzoyl)-3,6-dihydro-, ethyl ester (CA INDEX NAME)

847865-40-1 CAPLUS CN

Spiro[azepino[4,5-b]indole-1(2H),1'-cyclopropane]-5-carboxylic acid, 3-(3,4-difluorobenzoyl)-3,6-dihydro-, 1-methylethyl ester (CA INDEX NAME)

1088713-88-5 CAPLUS CN

Pyrrolo[2,3-d]azepine-2,8-dicarboxylic acid, 6-(3,4-difluorobenzoyl)-1,4,5,6-tetrahydro-4,4-dimethyl-, 2,8-dimethyl-ester (CA INDEX NAME)

OS.CITING REF COUNT:

THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD (1 CITINGS)

L29 ANSWER 3 OF 27 CAPLUS COPYRIGHT 2011 ACS on STN

ACCESSION NUMBER: 2009:647976 CAPLUS

DOCUMENT NUMBER: 1,4,5,6-Tetrahydropyrrolo[2,3-d]azepines AND -imidazo[4,5-d]azepines as modulators of nuclear

receptor activity INVENTOR(S): Mehlmann, John Francis: Lundquist, Joseph Theodore, IV; Mahaney, Paige Erin; Crawley, Matthew Lantz; Kim, Callain Younghee

PATENT ASSIGNEE (S): Wyeth, John, and Brother Ltd., USA U.S. Pat. Appl. Publ., 26pp. SOURCE .

CODEN: DISTACO

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 20090137554	A1	20090528	US 2008-255216	20081021
PRIORITY APPLN. INFO.:			US 2007-999990P P	20071022
ASSIGNMENT HISTORY FOR	US PATEN	T AVAILABLE	IN LSUS DISPLAY FORMAT	
OTHER SOURCE (S):	CASREA	CT 151:1373	: MARPAT 151:1373	

AB Disclosed are chemical entities including compds. of Formula (I and pharmaceutically acceptable salts thereof, wherein X is chosen from CN, CF3, CF2H, S(0) nR8, and S(0) 2N(R9) R10; n is 1, 2 or 3; Y is chosen from CR11 and N: 2 is chosen from 0 and NH; R1 is chosen from optionally substituted alkyl, cycloalkyl, etc.; R2 is H or optionally substituted alkyl; R3 is chosen from -C(0)R12 and -C(0)N(R9)R10; R4, R5, R6 and R7 are independently chosen from H and optionally substituted alkyl; R8 is chosen from optionally substituted alkyl or cycloalkyl; R9 and R10 is chosen from H or optionally substituted anyl or heteroaryl, etc.; R11 is H or lower alkyl; R12 is H, optionally substituted aryl or heteroaryl, etc.); compns. comprising one or more such chemical entities; and methods of using one or more such chemical entities for modulating the activity of certain nuclear receptors (e.g., farnesoid X) or for the treatment or prevention of one or more symptoms of disease or disorder related to the activity of those receptors.

1158716-04-1P 1158716-05-2P 1158716-06-3P 1158716-07-4P 1158716-08-5P 1158716-09-6P

1158716-10-9P 1158716-11-0P 1158716-12-1P

1158716-13-2P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(tetrahydropyrroloazepines and -imidazoazepines as modulators of farnesoid X receptors for disease treatment) 1158716-04-1 CAPLUS

RN CN Pyrrolo[2,3-d]azepine-8-carboxylic acid,

2-cyano-6-(3,4-difluorobenzoyl)-1,4,5,6-tetrahydro-4,4-dimethyl-, 1-methylethyl ester (CA INDEX NAME)

1158716-05-2 CAPLUS

CN Pyrrolo[2,3-d]azepine-8-carboxylic acid.

2-cyano-6-(cyclohexylcarbonyl)-1,4,5,6-tetrahydro-4,4-dimethyl-, 1-methylethyl ester (CA INDEX NAME)

RN 1158716-06-3 CAPLUS

Pyrrolo[2,3-d]azepine-8-carboxylic acid. CN

2-cyano-6-(3-fluorobenzoyl)-1,4,5,6-tetrahydro-4,4-dimethyl-,

1-methylethyl ester (CA INDEX NAME)

RN 1158716-07-4 CAPLUS CN Pyrrolo[2,3-d]azepin

Pyrrolo[2,3-d]azepine-8-carboxylic acid, 2-cyano-6-(4-fluorobenzoyl)-1,4,5,6-tetrahydro-4,4-dimethyl-, 1-methylethyl ester (CA INDEX NAME)

RN 1158716-08-5 CAPLUS CN Pyrrolo[2,3-d]azepin

N Pyrrolo[2,3-d]azepine-8-carboxylic acid, 2-cyano-6-(4-cyanobenzoyl)-1,4,5,6-tetrahydro-4,4-dimethyl-, 1-methylethyl ester (CA INDEX NAME)

RN 1158716-09-6 CAPLUS

CN Pyrrolo[2,3-d]azepine-8-carboxylic acid, 6-(3-chlorobenzoyl)-2-cyano-1,4,5,6-tetrahydro-4,4-dimethyl-, 1-methylathyl estor (CA INDEX NAME)

RN 1158716-10-9 CAPLUS CN Pyrrolo[2,3-d]azepin

Pyrrolo[2,3-d]azepine-8-carboxylic acid, 2-cyano-1,4,5,6-tetrahydro-4,4-dimethyl-6-(2-thienylcarbonyl)-, 1-methylethyl ester (CA INDEX NAME)

RN 1158716-11-0 CAPLUS

CN Pyrrolo [2,3-d] azepine-8-carboxylic acid, 2-cyano-1,4,5,6-tetrahydro-4,4-dimethyl-6-[3-(trifluoromethyl) benzoyl]-, 1-methylethyl ester (CA INDEX NAME).

RN 1158716-12-1 CAPLUS

NN 130-10-12-1 Charles of the Archive transfer of t

RN 1158716-13-2 CAPLUS CN Spiro(4H-pyran-4,4'(1'H)-pyr

Spiro[4H-pyran-4,4'(1'H)-pyrrolo[2,3-d]azepine]-8'-carboxylic acid, 2'-cyano-6'-(3,4-difluorobenzoyl)-2,3,5,5',6,6'-hexahydro-, 1-methylethyl ester (CA INDEX NAME)

IT 1155659-03-2P 1158716-22-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (tetrahydropyrroloazepines and -imidazoazepines as modulators of

(tetrahydropyrroloazepines and -imidazoazepines as modulators of farnesoid X receptors for disease treatment)

RN 1155659-03-2 CAPLUS

CN Pyrrolo[2,3-d] azepine-8-carboxylic acid, 2-cyano-1,4,5,6-tetrahydro-4,4-dimethyl-, 1-methylethyl ester (CA INDEX NAME)

RN 1158716-22-3 CAPLUS

CN Spiro[4H-pyran-4,4'(1'H)-pyrrolo[2,3-d]azepine]-8'-carboxylic acid,

2'-cyano-2,3,5,5',6,6'-hexahydro-, 1-methylethyl ester (CA INDEX NAME)

OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD (1 CITINGS)

10/565,702

L29 ANSWER 4 OF 27 CAPLUS COPYRIGHT 2011 ACS on STN

2009:615712 CAPLUS

ACCESSION NUMBER: DOCUMENT NUMBER:

150:555909 1,4,5,6,7,8-Hexahydro-pyrrolo[2,3-d]azepines and -imidazo[4,5-d]azepines as modulators of nuclear receptor activity

INVENTOR(S): Mehlmann, John Francis; Lundquist, Joseph Theodore, IV; Mahaney, Paige Erin; Crawley, Matthew Lantz; Kim, Callain Younghee

PATENT ASSIGNEE (S): Wyeth, John, and Brother Ltd., USA U.S. Pat. Appl. Publ., 25pp. SOURCE .

CODEN: DISTACO DOCUMENT TYPE: Patent

LANGUAGE: English FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO. KIND DATE APPLICATION NO. DATE US 20090131409 A1 20090521 US 2008-255232 20081021 US 2007-11P PRIORITY APPLN. INFO.: 20071022 ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT

CASREACT 150:555909: MARPAT 150:555909

OTHER SOURCE (S):

AB Disclosed are chemical entities including compds. of Formula (I and pharmaceutically acceptable salts thereof, wherein X is chosen from CN, CF3, CF2H, S(0) nR8, and S(0) 2N(R9) R10; n is 1, 2 or 3; Y is chosen from CR11 and N: Z is chosen from O and NH; R1 is chosen from optionally substituted alkyl, cycloalkyl, etc.; R2 is H or optionally substituted alkyl; R3 is chosen from -C(0)R12 and -C(0)N(R9)R10; R4, R5, R6 and R7 are independently chosen from H and optionally substituted alkyl; R8 is chosen from optionally substituted alkyl or cycloalkyl; R9 and R10 is chosen from H or optionally substituted aryl or heteroaryl, etc.; R11 is H or lower alkyl; R12 is H, optionally substituted aryl or heteroaryl, etc.); compns. comprising one or more such chemical entities; and methods of using one or more such chemical entities for modulating the activity of certain nuclear receptors (e.g., farnesoid X) or for the treatment or prevention of one or more symptoms of disease or disorder related to the activity of those receptors.

TT 1155659-03-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

(Reactant or reagent)

(hexahydro-pyrroloazepines and -imidazoazepines as modulators of farnesoid X receptor activity for treatment of disease)

RN 1155659-03-2 CAPLUS

CN Pyrrolo[2,3-d]azepine-8-carboxylic acid,

Pyrio10[2,3-0]dzeplne-6-Carboxylic detd, 2-cyano-1,4,5,6-tetrahydro-4,4-dimethyl-, 1-methylethyl ester (CA INDEX NAME)

OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD (1 CITINGS)

L29 ANSWER 5 OF 27 CAPLUS COPYRIGHT 2011 ACS on STN

ACCESSION NUMBER: 2008:1457368 CAPLUS

DOCUMENT NUMBER: 150:16134
TITLE: Farnesold X receptor (FXR) agonists for reducing lectin-like oxidized low-density lipoprotein receptor

INVENTOR(S):

1 (LOX-1) expression, and therapeutic use
Harnish, Douglas; Zhang, Songwen
PATENT ASSIGNEE(S):
Wyoth, John, and Brother Ltd., USA
SOURCE:
U.S. Pat. Appl. Pabl., Zépp.

SOURCE: U.S. Pat. Appl. Publi CODEN: USXXCO

LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO. KIND DATE APPLICATION NO. DATE
US 20080300235 Al 20081204 US 2008-130322 20088530
PRIORITY APPLN, 1NFO.: US 2007-924822P P 20070601

ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT AB The invention provides methods for treating at least one disease state characterized by elevated expression of the lectin-like oxidized low-d.

lipoprotein receptor 1 (LOX-1) in a patient with farmesoid X receptor (FXR) agonists. Also provided are methods for reducing expression of LOX-1 in a cell with FXR agonists.

IT 629664-83-1 837429-85-3,

6-(4-Fluorobenzoyl)-3,6,7,8-tetrahydroimidazo(4,5-d)azepine-4-carboxylic acid ethyl ester 837429-86-4, 6-(3,4-Difluorobenzoyl)-5,6-dihydro-4H-thieno(2,3-d)azepine-8-carboxylic

acid ethyl ester 837429-88-6, 3-(4-Fluorobenzoyl)1,2,3,6,7,8,9,10-octahydroazepino[4,5-b]indole-5-

carboxylic acid ethyl ester 837429-89-7,
3-(4-Fluorobenzoyl)-1,1-dimethyl-1,2,3,6,7,8,9,10-octahydroazepino[4,5-

blindole-5-carboxylic acid ethyl ester 837429-90-0 837429-91-1, 6-(3,4-Difluorobenzoyl)-4,4-dimethyl-1,4,5,6-

tetrahydropyrrolo[2,3-d]azepine-2,8-dicarboxylic acid diethyl ester 837429-92-2 837429-93-3 847865-38-7

847865-39-8 847865-40-1 1088713-88-5

RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(FXR agonists for reducing LOX-1 expression, and therapeutic use) RN 629664-83-1 CAPLUS

CN Spiro[azepino[4,5-b]indole-1(2H),1'-cyclopentane]-5-carboxylic acid, 3-(3,4-difluorobenzoyl)-3,6-dihydro-, ethyl ester (CA INDEX NAME)



10/565,702

RN 837429-85-3 CAPLUS

CN Imidazo[4,5-d]azepine-4-carboxylic acid,

6-(4-fluorobenzoyl)-3,6,7,8-tetrahydro-, ethyl ester (CA INDEX NAME)

RN 837429-86-4 CAPLUS

CN 4H-Thieno[2,3-d]azepine-8-carboxylic acid, 6-[3,4-difluorobenzovl)-5,6-dihydro-, ethyl ester (CA INDEX NAME)

RN 837429-88-6 CAPLUS

CN Azenino[4.5-blindole-5-carboxvlic acid.

3-(4-fluorobenzoyl)-1,2,3,6,7,8,9,10-octahydro-, ethyl ester (CA INDEX NAME)

RN 837429-89-7 CAPLUS

CN Azepino (4,5-b) indole-5-carboxylic acid,

3-(4-fluorobenzoyl)-1,2,3,6,7,8,9,10-octahydro-1,1-dimethyl-, ethyl ester (CA INDEX NAME)

RN 837429-90-0 CAPLUS

CN 4H-Thieno[2,3-d]azepine-8-carboxylic acid, 6-(3,4-difluorobenzoyl)-5,6-dihydro-4,4-dimethyl-, ethyl ester (CA INDEX NAME)

RN 837429-91-1 CAPLUS

CN Pyrrolo[2,3-d]azepine-2,8-dicarboxylic acid, 6-(3,4-difluorobenzoyl)-1,4,5,6-tetrahydro-4,4-dimethyl-, 2,8-diethyl ester (CA INDEX NAME)

RN 837429-92-2 CAPLUS

CN Pyrrolo[2,3-d]azepine-2,8-dicarboxylic acid, 6-(3,4-difluorobenzoyl)-1,4,5,6-tetrahydro-4,4-dimethyl-, 2-ethyl 8-(1-methylathyl) estor (CA INDEX NAME)

RN 837429-93-3 CAPLUS CN Pyrrolo[2,3-d]azenia

Pyrrolo[2,3-d]azepine-2,8-dicarboxylic acid, 6-(3,4-difluorobenzoyl)-1,4,5,6-tetrahydro-1,4,4-trimethyl-, 2-ethyl 8-(1-methylethyl) ester (CA INDEX NAME)

RN 847865-38-7 CAPLUS

CN Spiro[azepino[4,5-b]indole-1(2H),1'-cyclobutane]-5-carboxylic acid, 3-(3,4-difluorobenzoyl)-3,6-dihydro-, ethyl ester (CA INDEX NAME)

RN 847865-39-8 CAPLUS

CN Spiro[azepino (4,5-b]indole-1(2H),1'-cyclopropane]-5-carboxylic acid, 3-(3,4-difluorobenzoyl)-3,6-dihydro-, ethyl ester (CA INDEX NAME)

RN 847865-40-1 CAPLUS
CN Spiro[azepino[4,5-b]indole-1(2H),1'-cyclopropane]-5-carboxylic acid,
3-(3,4-df[luorobenzoyl)-3,6-dihydro-, 1-methylethyl ester (CA INDEX NAME)

RN 1088713-88-5 CAPLUS CN Pyrrolo[2,3-d]azepine-2,8-dicarboxylic acid,

N Pyrrolo[2,3-d]azepine-2,8-dicarboxylic acid, 6-(3,4-difluorobenzoyl)-1,4,5,6-tetrahydro-4,4-dimethyl-, 2,8-dimethylester (CA INDEX NAME)

1

OS.CITING REF COUNT:

THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD (1 CITINGS)

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L29 ANSWER 6 OF 27 CAPLUS COPYRIGHT 2011 ACS on STN
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ACCESSION NUMBER: 2008:1455334 CAPLUS

DOCUMENT NUMBER: 150:16058
TITLE: FXR agonists for the treatment of malignancies

INVENTOR(S): Hartman, Helen B.; Evans, Mark J.
PATENT ASSIGNEE(S): Wyeth, John, and Brother Ltd., USA
SOURCE: U.S. Pat. Appl. Publ. . 25pp.

CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English

LANGUAGE: E
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

AB Provided are certain methods of treating malignancies with farnesoid X receptor agenists. Also provided are certain methods of inducing RECK game expression with farnesoid X receptor agenists and methods of reducing

gene application with minesold at least one feature of a cell with farnesold X receptor agonists.

T 629664-83-1 837429-85-3,
6-(4-FUlurobeagov)1-3,6,7,8-tetrahydroimidazo[4,5-Dlazepine-4-carboxylic

acid ethyl ester 837429-86-4, 6-(3,4-Difluorobenzoyl)-5,6-dihydro-4H-thieno[2,3-D]azepine-8-carboxylic

acid ethyl ester 837429-88-6, 3-(4-Pluorobenzoyl)1,2,3,6,7,8,9,10-octahydroazepino[4,5-b]indole-5-

carboxylic acid ethyl ester 837429-89-7, 3-(4-Fluorobenzoyl)-1,1-dimethyl-1,2,3,6,7,8,9,10-octahydroazepino[4,5-

b)indole-5-carboxylic acid ethyl ester 837429-90-0, 6-(3,4-Difluorobenzoyl)-4,4-dimethyl-5,6-dihydro-4H-thieno(2,3-d)azepine-8-

carboxylic acid ethyl ester 837429-91-1, 6-(3,4-Difluorobenzoyl)-4,4-dimethyl-1,4,5,6-tetrahydropyrrolo[2,3-d]azepine-2,8-dicarboxylic acid diethyl ester 837429-92-2

837429-93-3 847865-38-7 847865-39-8

847865-40-1 1088713-88-5

RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(farmesoid X receptor agonists for treatment of malignancies by inducing RECK gene expression)
RN 629664-83-1 CAPEUS

CN Spiro[azepino[4,5-b]indole-1(2H),1'-cyclopentane]-5-carboxylic acid, 3-(3,4-difluorobenzoyl)-3,6-dihydro-, ethyl ester (CA INDEX NAME)

10/565,702

RN 837429-85-3 CAPLUS

CN Imidazo[4,5-d]azepine-4-carboxylic acid,

6-(4-fluorobenzoyl)-3,6,7,8-tetrahydro-, ethyl ester (CA INDEX NAME)

RN 837429-86-4 CAPLUS

CN 4H-Thieno[2,3-d]azepine-8-carboxylic acid, 6-(3,4-difluorobenzovl)-5,6-dihydro-, ethyl ester (CA INDEX NAME)

RN 837429-88-6 CAPLUS

CN Azenino[4.5-blindole-5-carboxvlic acid.

NAME)

RN 837429-89-7 CAPLUS

CN Azepino (4,5-b) indole-5-carboxylic acid,

3-(4-fluorobenzoyl)-1,2,3,6,7,8,9,10-octahydro-1,1-dimethyl-, ethyl ester (CA INDEX NAME)

RN 837429-90-0 CAPLUS CN 4H-Thieno[2.3-d]azer

4H-Thieno[2,3-d]azepine-8-carboxylic acid, 6-(3,4-difluorobenzoyl)-5,6-dihydro-4,4-dimethyl-, ethyl ester (CA INDEX NAME)

RN 837429-91-1 CAPLUS

CN Pyrrolo[2,3-d]axepine-2,8-dicarboxylic acid, 6-(3,4-difluorobenzoyl)-1,4,5,6-tetrahydro-4,4-dimethyl-, 2,8-diethyl ester (CA INDEX NAME)

RN 837429-92-2 CAPLUS

CN Pyrrolo[2,3-d]azepine-2,8-dicarboxylic acid, 6-(3,4-difluorobenzoyl)-1,4,5,6-tetrahydro-4,4-dimethyl-, 2-ethyl 8-(1-methylathyl) estor (CA INDEX NAME)

RN 837429-93-3 CAPLUS

CN Pyrrolo[2,3-d]azepine-2,8-dicarboxylic acid, 6-(3,4-difluorobenzoyl)-1,4,5,6-tetrahydro-1,4,4-trimethyl-, 2-ethyl 8-(1-methylethyl) ester (CA INDEX NAME)

RN 847865-38-7 CAPLUS

CN Spiro[azepino[4,5-b]indole-1(2H),1'-cyclobutane]-5-carboxylic acid, 3-(3,4-difluorobenzoyl)-3,6-dihydro-, ethyl ester (CA INDEX NAME)

RN 847865-39-8 CAPLUS

CN Spiro[azepino 4,5-b]indole-1(2H),1'-cyclopropane]-5-carboxylic acid, 3-(3,4-difluorobenzoyl)-3,6-dihydro-, ethyl ester (CA INDEX NAME)

847865-40-1 CAPLUS CN Spiro[azepino[4,5-b]indole-1(2H),1'-cyclopropane]-5-carboxylic acid, 3-(3,4-difluorobenzoyl)-3,6-dihydro-, 1-methylethyl ester (CA INDEX NAME)

1088713-88-5 CAPLUS RN CN

Pyrrolo[2,3-d]azepine-2,8-dicarboxylic acid, 6-(3,4-difluorobenzoyl)-1,4,5,6-tetrahydro-4,4-dimethyl-, 2,8-dimethyl ester (CA INDEX NAME)

1

OS.CITING REF COUNT:

THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD (1 CITINGS)

L29 ANSWER 7 OF 27 CAPLUS COPYRIGHT 2011 ACS on STN

ACCESSION NUMBER: 2005:220132 CAPLUS

DOCUMENT NUMBER: 142:298092

TITLE: Preparation of azepino[4,5-b]indole derivatives as modulators of nuclear receptors
INVENTOR(S): Busch, Brett; Flatt, Brenton T.; Gu, Xiao-Hui; Martin,

Richard; Mohan, Raju; Wang, Tie-Lin; Wa, Jason H.
X-Ceptor Therapoutics Inc., USA; Exelixis, Inc.
SOURCE: U.S. Pat. Appl. Publ., 106 pp., Cont.-in-part of U.S.

Ser. No. 447,302. CODEN: USXXCO

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 2 PATENT INFORMATION:

PAT	PENT	NO.			KIN	D	DATE			APPI	LICAT	ION	NO.		D	ATE		
US	US 20050054634				A1 200			050310			2003-	8954		20031202				
US	7595311				B2 20090929													
US	2004	20040023947								US 2003-447302						0030	527	
US	7485	7485634					2009	0203										
AU	2004	2004297198				A1 20050623					2004-	2971	20041201					
CA	2555279				A1	2005	0623		CA 2004-2555279						20041201			
WO	2005	2005056554				A2 20050623					2004-	US40	352		20041201			
WO	2005	0565	54		A3		2005	0818										
	W:										BG,							
		CN,	CO,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	EG,	ES,	FI,	GB,	GD,	
		GE,	GH,	GM,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	KE,	KG,	KP,	KR,	KZ,	LC,	
											MK,							
		NO,	NZ,	OM,	PG,	PH,	PL,	PT,	RO,	RU,	SC,	SD,	SE,	SG,	SK,	SL,	SY,	
											UZ,							
	RW:										SL,							
											BE,							
											IT,							
							BF,	BJ,	CF,	CG,	CI,	CM,	GA,	GN,	GQ,	GW,	ML,	
				SN,	TD,													
EP	1692									EP 2004-812795								
	R:										IT,							
						FI,	RO,	MK,	CY,	ΑL,	TR,	BG,	CZ,	EE,	HU,	PL,	SK,	
			HR,	IS,														
	1914				A						2004-		20041201					
	2004				A						2004-		20041201					
	2007										2006-		20041201					
	5481												20041201					
ZA	2006	0043	52		A		2008				2006-		20060529					
MX	2006	0061	40		A	A 20061110				MX 2006-6140					20060531			
IN	2006	KN01	497		A			0504		IN 2006-KN1497					20060601			
	MX 2006006140 IN 2006KN01497 KR 2006124662							1205		KR 2006-7013217								
NO 2006003080				A.			0823							2	0060	703		
US 20090326218 US 20100173824				A1		2009				2009-				2	0090	129		
					A1		2010	0708			2009-							
	2010				A		2010	1014			2010-					0100		
ORIT	Y APP	LN.	INFO	. :							2002-							
											2003-				N2 2			
											2004-				A3 2			
										05 2	2003-	8954	31.		A 2	0031	202	

WO 2004-US40352 W 20041201

ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT OTHER SOURCE (S): CASREACT 142:298092; MARPAT 142:298092

AB The title compds. (I) [R1 = -C(J)OR14, -C(J)SR14, (un)substituted -C(J)NH2; J - O. S. (un) substituted NH; R2 - H. halo, (un) substituted alkyl; R3 = -C(O)R9; R4, R5, R6 and R7 are together selected from (a), (b), etc. below: (a) R4, R5 = H or halo and R6, R7 = halo, each (un) substituted alkyl, alkenyl, alkynyl, cycloalkyl, cycloalkylalkyl, heterocyclyl, heterocyclylalkyl, aryl, aralkyl, heteroaryl, or heterogralkyl, etc.; or R6 and R7, together with the carbon atom to which they are attached, form each (un) substituted cycloalkyl, heterocyclyl, cycloalkenyl, alkylidene, cycloalkylidene, heterocyclylidene, aralkylidene or substituted heteroaralkylidene; (b) R4, R5 = halo, each (un) substituted alkyl, alkenyl, alkynyl, cycloalkyl, cycloalkylalkyl, heterocyclyl, heterocyclylalkyl, aryl, heteroaryl, or heteroaralkyl, etc.; or R4 and R5, together with the carbon atom to which they are attached, form (un) substituted cycloalkyl, heterocyclyl, cycloalkenyl, alkylidene, cycloalkylidene, heterocyclylidene, aralkylidene or heteroaralkylidene, and R6, R7 = H or halo; R8a, R8b, R8c, R8d = H, halo, pseudohalo, cyano, azido, amidino, quanidino, each (un) substituted alkyl, alkenyl, alkynyl, cycloalkyl, cycloalkylalkyl, heterocyclyl, heterocyclylalkyl, aryl, aralkyl, heteroaryl, or heteroaralkyl, etc.; R14 - each (un) substituted alkyl, alkenyl, alkynyl, cycloalkyl, cycloalkylalkyl, heterocyclyl, heterocyclylalkyl, etc.1 are prepared These compds, modulate nuclear receptors, in particular farmesoid X receptor and are agonists, partial agonists, inverse agonists, partial antagonists, or antagonists of farnesoid X receptor. They are useful for the treatment, prevention, or amelioration of one or more symptoms of disease or disorder directly or indirectly related to the activity of the above receptors, including hyperlipidemia, hypercholesterolemia, hypertriglyceridemia, dyslipidemia, lipodystrophy, atherosclerosis, atherosclerotic disease, atherosclerotic disease events, atherosclerotic cardiovascular disease, Syndrome X, diabetes mellitus, type II diabetes, insulin insensitivity, hyperqlycemia, cholestasis and obesity. Thus, to a solution of Et 1,2,3,6-tetrahydroazepino[4,5-b]indole-5-carboxylate (52 mg, 0.2 mmol) in CH2C12 was added 4-fluorobenzovl chloride (36 µL, 0.2 mmol) and TEA (56 μL, 0.4 mmol) and the mixture was shaken overnight at 20°, treated with Trisamine resin (50 mg), and shaken for 2 h at 20°. The resin was removed by filtration through a Florisil cartridge. Evaporation of solvent gave a crude product, which was purified by trituration with methanol to give Et 3-(4-fluorobenzoyl)-1,2,3,6-tetrahydroazepino[4,5-b]indole-5carboxylate. Et 3-(3,4-difluorobenzovl)-1-methyl-1,2,3,6tetrahydroazepino[4,5-blindole-5-carboxylate was administered daily by

oral gage for 7 days to young adult male mice. Plasma total cholesterol and triglyceride levels were significantly lowered. 629662-33-5P 629664-84-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

(Reactant or reagent) (intermediate; preparation of azepino 4.5-blindole derivs, as modulators of

nuclear receptors, in particular farmesoid X receptor) RN 629662-33-5 CAPLUS CN

1H-Benzofuro[2,3-d]azepine-5-carboxylic acid, 2,3-dihydro-, ethyl ester (CA INDEX NAME)

RN 629664-84-2 CAPLUS

Spiro[azepino[4,5-b]indole-1(2H),1'-cyclopentane]-5-carboxylic acid, CN 3,6-dihydro-, ethyl ester (CA INDEX NAME)

IT 629662-32-4P 629662-34-6P 629663-80-5P 629664-83-1P 847865-38-7P 847865-39-8P

847865-40-1P RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES

(Uses) (preparation of azepino[4,5-b]indole derivs. as modulators of nuclear receptors, in particular farmesoid X receptor)

629662-32-4 CAPLUS

RN CN 1H-Benzofuro[2,3-d]azepine-5-carboxylic acid,

3-(3,4-difluorobenzoyl)-2,3-dihydro-, ethyl ester (CA INDEX NAME)

RN 629662-34-6 CAPLUS

GN 1H-[1]Benzothieno[2,3-d]azepine-5-carboxylic acid, 3-(3,4-difluorobenzoyl)-2,3-dihydro-, ethyl ester (CA INDEX NAME)

RN 629663-80-5 CAPLUS
CN Spiro(azepino[4,5-b]indole-1(2H),2'-[1,3]dioxolane]-5-carboxylic acid,
3-(4-fluorobenzoyl)-3,6-dihydro-, ethyl ester (CA INDEX NAME)

RN 629664-83-1 CAPLUS

CN Spiro[azepino[4,5-b]indole-1(2H),1"-cyclopentane]-5-carboxylic acid, 3-(3,4-difluorobenzoyl)-3,6-dihydro-, ethyl ester (CA INDEX NAME)

RN 847865-38-7 CAPLUS
CN Spiro(azepino[4,5-b]indole-1(2H),1'-cyclobutane]-5-carboxylic acid,
3-(3,4-difluorobenzoyl)-3,6-dihydro-, ethyl ester (CA INDEX NAME)

RN 847865-39-8 CAPLUS CN Spiro(azepino(4.5-b)indole

CN Spiro[azepino[4,5-b]indole-1(2H),1'-cyclopropane]-5-carboxylic acid, 3-(3,4-difluorobenzoyl)-3,6-dihydro-, ethyl ester (CA INDEX NAME)



RN 847865-40-1 CAPLUS CN Spiro(azepino(4.5-b)

Spiro[azepino[4,5-b]indole-1(2H),1'-cyclopropane]-5-carboxylic acid, 3-(3,4-difluorobenzoyl)-3,6-dihydro-, 1-methylethyl ester (CA INDEX NAME)

OS.CITING REF COUNT: 9 THERE ARE 9 CAPLUS RECORDS THAT CITE THIS RECORD (11 CITINGS)

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ACCESSION NUMBER: 2005:99333 CAPLUS
DOCUMENT NUMBER: 142:198048
TITLE: Arepine derivatives as pharmaceutical agents, specifically as farnesoid X receptor ligands, and their preparation, pharmaceutical compositions, and
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their preparation, pharmaceutical compositions use in the treatment of lipid disorders, atherosclerosis, and diabetes

INVENTOR(S): Martin, Richardy Mang, Tio-Lin; Flatt, Brenton T.; Gu, Xiao-Hai
PATENT ASSIGNEE(S): X-Coptor Therapeutics Inc., USA

PATENT ASSIGNEE(S): X-Ceptor Therapeutics Inc., USA
SOURCE: PCT Int. Appl., 133 pp.
CODEN: FIXXD2
DOCUMENT TYPE: Patent

L29 ANSWER 8 OF 27 CAPLUS COPYRIGHT 2011 ACS on STN

LANGUAGE: English FAMILY ACC. NUM. COUNT: 1 PATENT INFORMATION:

> PATENT NO. KIND DATE APPLICATION NO. DATE WO 2005009387 A2 20050203 WO 2004-US23745 20040723 A3 20060302 WO 2005009387 W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI. SK. TR. BF. BJ. CF. CG. CI. CM. GA. GN. GO. GW. ML. MR. NE. SN. TD. TG AU 2004259009 20050203 AU 2004-259009 20040723 CA 2004-2532798 CA 2532798 20040723 20060426 EP 2004-779004 20040723 EP 1648408 R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK, HR BR 2004012262 A 20060919 BR 2004-12262 20040723 CN 1852748 20061025 CN 2004-80027076 20040723 JP 2006528637 T 20061221 JP 2006-521272 20040723 JP 4679517 B2 20110427 KR 2006052867 A 20060519 KR 2006-7001566 20060123 MX 2006000875 A 20060907 MX 2006-875 20060123 NO 2006000871 A 20060424 NO 2006-871 20060222 US 20070015746 A1 20070118 US 2006-565702 20060913 US 2003-489854P P 20030723

PRIORITY APPLN. INPO.:

US 2003-489854P P 20030723

O 2004-US23745 W 20040723

ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT

OTHER SOURCE (S):

CASPEACT 142:199048 MARPET 142:199048

AB Compds., compns., and methods are provided for modulating the activity of farnesoid X receptors, and for the treatment, prevention, or amelioration of one or more symptoms of diseases or disorders related to the activity of the receptors. In particular, compds. I are disclosed [wherein: X = 0, S(O)0-2, NH or its alkyl, acylated, oxyacylated, or sulfonylated derivs.; Y = (un) substituted CH or N: Z = (un) substituted CH or N: or YZ bond is fused to a carbo- or heterocyclic ring, but not benze or naphtho; R1, R2, R4-R7 - H, halo, (un)substituted alk(en/yn)yl, (hetero)aryl, numerous functional groups; R3 = H, (un) substituted alk(en/yn)yl, (hetero)aryl, numerous functional groups; R4R5 and/or R6R7 may form oxo, thioxo, (un) substituted imino or oxime or hydrazone, or an exocyclic double bond; or R4R5, R4R6, R4R7, R5R6, R5R7, and/or R6R7 may form ring(s); including isomer(s), solvates, polymorphs, prodrugs, and pharmaceutically acceptable salts]. Fifteen synthetic examples and several biol. examples are given. For instance, thiophene-3-acetonitrile was converted to invention compound II in four steps: (1) di-α-methylation using NaH and MeI in DMF; (2) reduction of the nitrile to a primary amine using LiAlH4; (3) cyclocondensation of the amine with Et bromopyruyate to form the azepine ring; and (4) N-acylation using 3.4-difluorobenzovl chloride. II exhibited agonist activity at 100 nM or less, with > 100% efficacy (vs. CDCA), as measured in a co-transfection assay using full length human

farnesoid X receptor. B37429-84-2P, 3,6,7,8-Tetrahydroimidazo[4,5-d]azepine-4carboxvlic acid ethyl ester

RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(drug candidate; preparation of azepine derivs. as farnesoid X receptor ligands for treatment of lipid disorders, atherosclerosis, and diabetes)

RN 837429-84-2 CAPLUS
CN Imidazo[4,5-d]azepine-4-carboxylic acid, 3,6,7,8-tetrahydro-, ethyl ester (CA INDEX NAME)

Page 71

IT 837429-85-3P, 6-(4-Pluorobenzoyl)-3,6.7,8-tetrahydroimidazo[4,5-dlazoplned-earboylic acid ethyl ester 837429-86-79,6-6,3,4-0!fluorobenzoyl)-5,6-dihydro-4H-thleno[2,3-d]azepine-8-carboxylic acid ethyl ester 837429-88-79.

acid etnyl ester 83/429-88-PP, 3-(4-Fluorobenzoyl)-1,2,3,6,7,8,9,10-octahydroazepino[4,5-b]indole-5carboxylic acid ethyl ester 837429-89-7P,

3-(4-Pluorobenzoyl)-1,1-dimethyl-1,2,3,6,7,8,9,10-octahydroazepino[4,5-b]indole-5-carboxylic acid ethyl ester 837429-90-06-6-(3,4-b]fluorobenzoyl)-4,4-dimethyl-5,6-dihydro-4H-thieno[2,3-d]azepine-8-6-(3,4-b]fluorobenzoyl)-4,4-dimethyl-5,6-dihydro-4H-thieno[2,3-d]azepine-8-6-(3,4-b]fluorobenzoyl)-4,4-dimethyl-5,6-dihydro-4H-thieno[2,3-d]azepine-8-6-(3,4-b)fluorobenzoyl)-4,4-dimethyl-5,6-dihydro-4H-thieno[2,3-d]azepine-8-6-(3,4-b)fluorobenzoyl)-4,5-dimethyl-5,6-dihydro-4H-thieno[2,3-d]azepine-8-6-(3,4-b)fluorobenzoyl)-4,5-dimethyl-5,6-dihydro-4H-thieno[2,3-d]azepine-8-6-(3,4-b)fluorobenzoyl-4,5-dimethyl-5,6-dihydro-4H-thieno[2,3-d]azepine-8-6-(3,4-b)fluorobenzoyl-4,5-dimethyl-5,6-dihydro-4H-thieno[2,3-d]azepine-8-6-(3,4-b)fluorobenzoyl-4,5-dimethyl-5,6-dihydro-4H-thieno[2,3-d]azepine-8-6-(3,4-b)fluorobenzoyl-4,5-dimethyl-5,6-dihydro-4H-thieno[2,3-d]azepine-8-6-(3,4-b)fluorobenzoyl-4,5-dihydro-4H-thieno[2,3-d]azepine-8-6-(3,4-b)fluorobenzoyl-4,5-dihydro-4H-thienopyl-4,5-dihydro-4H-thi

carboxylic acid ethyl ester 837429-91-1P, 6-(3,4-0)floorobenzoyl-4,4-diaethyl-1,4,5,6-tetrahydropyrrolo[2,3-d]azepine-2,8-dicarboxylic acid diethyl ester 837429-92-2P, 6-(3,4-0)floorobenzoyl-4,4-diaethyl-1,4,5,6-tetrahydropyrrolo[2,3-diaethyl-1,4,5,6-tetrahydropyrrolo[2,3-diaethyl-1,4,5].

dlazepine-2,8-dicarboxylic acid 2-ethyl ester 8-isopropyl ester 83/429-93-39, 6-(3,4-Difluorobenzoyl)-1,4,4-trimethyl-1,4,5,6tetrahydropyrrolo[2,3-d]azepine-2,8-dicarboxylic acid 2-ethyl ester 8-isopropyl ester

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(drug candidate; preparation of szepine derivs. as farnesoid X receptor ligands for treatment of lipid disorders, atherosclerosis, and diabetes)

RN 837429-85-3 CAPLUS

CN Imidazo[4,5-d]azepine-4-carboxylic acid,

6-(4-fluorobenzoyl)-3,6,7,8-tetrahydro-, ethyl ester (CA INDEX NAME)

RN 837429-86-4 CAPLUS

CN 4H-Thieno[2,3-d]azepine-8-carboxylic acid, 6-(3,4-difluorobenzovl)-5,6-dihydro-, ethyl ester (CA INDEX NAME)

RN 837429-88-6 CAPLUS

CN Azepino[4,5-b]indole-5-carboxylic acid, 3-(4-fluorobenzoyl)-1,2,3,6,7,8,9,10-octahydro-, ethyl ester (CA INDEX NAME)

RN 837429-89-7 CAPLUS

CN Azepino[4,5-b]indole-5-carboxylic acid, 3-(4-fluorobenzoyl)-1,2,3,6,7,8,9,10-octahydro-1,1-dimethyl-, ethyl ester (CA INDEX NAME)

RN 837429-90-0 CAPLUS CN 4H-Thieno[2,3-d]azer

N 4H-Thieno[2,3-d]azepine-8-carboxylic acid, 6-(3,4-difluorobenzoyl)-5,6-dihydro-4,4-dimethyl-, ethyl ester (CA INDEX NAME)

RN 837429-91-1 CAPLUS CN Pyrrolo[2,3-d]azenia

Pyrrolo[2,3-d]azepine-2,8-dicarboxylic acid, 6-(3,4-difluorobenzoyl)-1,4,5,6-tetrahydro-4,4-dimethyl-, 2,8-diethyl ester (CA INDEX NAME)

RN 837429-92-2 CAPLUS

CN Pyrrolo[2,3-d]azepine-2,8-dicarboxylic acid, 6-(3,4-difiuorobenzyl)-1,4,5,6-tetrahydro-4,4-dimethyl-, 2-ethyl 8-(1-methylethyl) ester (CA INDEX NAME)

RN 837429-93-3 CAPLUS

CN Pyrrolo[2,3-d]azepine-2,8-dicarboxylic acid,
6-(3,4-difluorobenzoyl)-1,4,5,6-tetrahydro-1,4,4-trimethyl-,2-ethyl
8-(1-methylethyl) ester (CA INDEX NAME)

IT 837429-95-5P, 5,6-Dihydro-4H-thieno[2,3-d]azepine-8-carboxylic acid ethyl ester 837429-96-6P, 4,4-Dimethyl-5,6-dihydro-4H-thieno[2,3-d]azepine-8-carboxylic acid ethyl ester 837430-02-1P, 4,4-Dimethyl-1,4,5,6-totrahydropyrrolo[2,3-d]azepine-8-8-dicarboxylic acid diethyl ester 837430-03-2P.

djazepine-2,8-dicarboxylic acid diethyl ester 837430-03-2P, 4,4-Dimethyl-1,4,5,6-tetrahydropyrrolo[2,3-d]azepine-2,8-dicarboxylic acid 2-ethyl ester 8-isopropyl ester 837430-05-4P,

1,4,4-Trimethyl-1,4,5,6-tetrahydropyrrolo[2,3-d]azepine-2,8-dicarboxylic acid 2-ethyl ester 8-isopropyl ester RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

(Reactant or reagent) (intermediate; preparation of azepine derivs. as farnesoid X receptor liquads for treatment of lipid disorders, atherosclerosis, and

diabetes) RN 837429-95-5 CAPLUS

CN 4H-Thieno[2,3-d]azepine-8-carboxylic acid, 5,6-dihydro-, ethyl ester (CA INDEX NAME)

RN 837429-96-6 CAPLUS

CN 4H-Thieno[2,3-d]azepine-8-carboxylic acid, 5,6-dihydro-4,4-dimethyl-, ethyl ester (CA INDEX NAME)

RN 837430-02-1 CAPLUS CN Pyrrolo[2,3-d]azeni

Pyrrolo[2,3-d]azepine-2,8-dicarboxylic acid, 1,4,5,6-tetrahydro-4,4-dimethyl-, 2,8-diethyl ester (CA INDEX NAME)

RN 837430-03-2 CAPLUS CN Pyrrolo[2,3-d]azepi

Pyrrolo[2,3-d]azepine-2,8-dicarboxylic acid, 1,4,5,6-tetrahydro-4,4-dimethyl-, 2-ethyl 8-(1-methylethyl) ester (CA INDEX NAME)

RN 837430-05-4 CAPLUS CN Pyrrolo[2,3-d]azenia

Pyrrolo[2,3-d]azepine-2,8-dicarboxylic acid, 1,4,5,6-tetrahydro-1,4,4-trimethyl-, 2-ethyl 8-(1-methylethyl) ester (CA INDEX NAME) 10/565,702



OS.CITING REF COUNT:

1

- 3 THERE ARE 3 CAPLUS RECORDS THAT CITE THIS RECORD (3 CITINGS)
- REFERENCE COUNT:
- THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

10/565,702

L29 ANSWER 9 OF 27 CAPLUS COPYRIGHT 2011 ACS on STN

ACCESSION NUMBER: 2004:848383 CAPLUS

DOCUMENT NUMBER: 142:6329
TITLE: Synthesis of the sterically fixed biliverdin

derivative bearing the Z-anti C/D-ring component
AUTHOR(S): Hammam, Mostafa A. S.; Murata, Yasue; Kinoshita,
Hideki; Inomata, Katsuhiko

Hideki; Inomata, Katsuhiko

CORPORATE SOURCE: Division of Material Sciences, Graduate School of

Natural Science and Technology, Kanazawa University,

Kanazawa, 920-1192, Japan SOURCE: Chemistry Letters (2004), 33(10), 1258-1259

CODEN: CMLTAG; ISSN: 0366-7022 PUBLISHER: Chemical Society of Japan

DOCUMENT TYPE: Journal

LANGUAGE: English OTHER SOURCE(S): CASREACT 142:6329

GI



AB A sterically locked biliverdin derivative I was synthesized by developing an efficient method for the preparation of Z-anti C/D-ring component toward investigation of the stereochem. and function of the phytochrome

chromophores. T 797050-86-3P 797050-93-2F

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (synthesis of the sterically fixed biliverdin derivative bearing the Z-anti

C/D-ring component) 797050-86-3 CAPLUS

Dipyrrolo[1,2-a:2',3'-d]azepine-3-propanoic acid,

8-ethyl-2-formyl-1,4,5,7-tetrahydro-9-methyl-7-oxo-, 2-propen-1-yl ester (CA INDEX NAME)

RN

CN

$$\mathbf{H}_2\mathbf{C} = \mathbf{C}\mathbf{H} - \mathbf{C}\mathbf{H}_2 - \mathbf{O} - \mathbf{C} - \mathbf{C}\mathbf{H}_2 - \mathbf{C}\mathbf{H}_2$$
 OHC

RN 797050-93-2 CAPLUS

CN Dipyrrolo[1,2-a:2',3'-d]azepine-3-propanoic acid,
2-[(1,1-dimethylethoxy)carbonyl]-8-ethyl-1,4,5,7-tetrahydro-9-methyl-7-oxo,2-propen-1-yl ester (CA INDEX NNBL)

OS.CITING REF COUNT:

- 12 THERE ARE 12 CAPLUS RECORDS THAT CITE THIS RECORD (12 CITINGS)
- REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L29 ANSWER 10 OF 27 CAPLUS COPYRIGHT 2011 ACS on STN

ACCESSION NUMBER: 2003:951028 CAPLUS

ACCESSION NUMBER: 2003:951028 CAPLU DOCUMENT NUMBER: 140:16715

TITLE: Preparation of azepinoindole and pyridoindole

derivatives as modulators of farnesoid X and/or orphan nuclear receptors

INVENTOR(S): Martin, Richard; Wang, Tie-Lin; Flatt, Brenton Todd;

Gu, Xiao-Hui; Griffith, Ronald
PATENT ASSIGNEE(S): X-Ceptor Therapeutics, Inc., USA

PATENT ASSIGNEE(S): A-Ceptor Therapeutics, inc. SOURCE: PCT Int. Appl., 268 pp.

DOCUMENT TYPE: Patent
LANGUAGE: English

OTHER SOURCE(S): MARPAT 140:16715

LANGUAGE: En FAMILY ACC. NUM. COUNT: 2

P	ATENT	INFOR	MATI	ON:														
	P#	TENT	NO.			KIN	D	DATE				LICAT				D	ATE	
	WC	WO 2003099821				A1 20031204												
		W:	AE,	AG,	AL,	AM,	AT,	AU,	AZ,	BA,	BB	, BG,	BR,	BY,	BZ,	CA,	CH,	CN,
			CO,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC	, EE,	ES,	FI,	GB,	GD,	GE,	GH,
												, KG,						
			LS,	LT,	LU,	LV,	MA,	MD,	MG,	MK,	MN	, Mid,	MX,	MZ,	NI,	NO,	NZ,	OM,
			PH,	PL,	PT,	RO,	RU,	SC,	SD,	SE,	SG	, SK,	SL,	TJ,	TM,	TN,	TR,	TT,
												, ZM,						
		RW:	GH,	GM,	KE,	LS,	MW,	MZ,	SD,	SL,	SZ	, TZ,	UG,	ZM,	ZW,	AM,	AZ,	BY,
												, CH,						
												, NL,						
												, GW,						
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		2003																
	EI	1532																
		R:										, IT,						PT,
												, TR,						
	JI	2005	5315	85		T		2005	1020		JP :	2004-	5074	78		2	0030	527
	JI	4646 2010	293			B2		2011	0309									
	JE	2010	2291	48		A		2010	1014		JP :	2010-	1356	20		2	0100	614
PRIORITY APPLN. INFO.:									US :	2002-	3835	74P		P 2	0020	524		
												2004-						
											WO:	2003-	US16	767		W 2	0030	527

AB The present invention is directed to azepinoindole and pyridoindole derivs, (shown as I and II; variables defined below; e.g. Et 1,2,3,6-tetrahydroazepino[4,5-b]indole-5-carboxylate). These compds. were used in pharmaceutical compns, and methods for modulating the activity of farnesoid X receptor and/or orphan nuclear receptors. A farnesoid X receptor/ECREx7 co-transfection assay and a TR-FRET assay were used to establish the EC50/IC50 values for potency and percent activity or inhibition for efficacy; efficacy defines the activity of a compound relative to a high control (chenodeoxycholic acid, CDCA) or a low control (DMSO/vehicle). Most of the compds. disclosed and tested exhibited activity in at least one of the assays (EC50 or IC50 <10 µM); most showed activity at <1 wM, e.g. Pr 3-(4-fluorobenzovl)-2-methyl-1.2.3.6-tetrahydroazepino[4.5-blindole-5carboxylate exhibited agonist activity <1 uM EC50 and >100 % efficacy and 8-(3-cyclopropyl-1-methylureido)-3-(4-fluorobenzoyl)-1,1-dimethyl-1,2,3,6-tetrahydroazepino[4,5-b]indole-5-carboxylic acid Et ester exhibited antagonist activity with IC50 <100 nM and 100 % inhibition. Although the methods of preparation are not claimed, 74 example prepns, of I and II and characterization data for many more I and II are included. For I and II: n = 0-4; A is -N(R9)-, -0- or -S(0)t- (t = 0-2); R1 and R2 = H, alkyl, alkenyl, alkynyl, aryl, heteroaryl, cycloalkyl, heterocyclyl, aralkyl, heteroaralkyl, -OR14, -SR14, -N(R15)R16, -N(R15)S(0)2R43; -N(R17)N(R15)R16, -N(R17)N(R15)S(0)2R43, -C(0)R18, -C(0)OR14, -C(S)OR14, -C(0) SR14, -C(0) N(R15) R16, -C(0) N(R15) S(0) 2R43, -C(0) N(R15) N:R16 and -C(0)N(R17)N(R15)R16; or -C(0)N(R17)N(R15)S(0)2R43; or R1 and R2, together with the atom to which they are attached, form a cycloalkyl, heterocyclyl, aryl, or heteroaryl ring. R3 is H, alkyl, alkenyl, alkynyl, cycloalkyl, aryl, or heteroaryl ring. R3 is H, alkyl, alkenyl, alkynyl, cycloalkyl, aryl, aralkyl, heteroaryl, heterocyclyl, heteroaralkyl, -C(0)R10, -C(0)R11); S(0)2R43, -C(0)R13)N(R11)R12, -C(0)N(R13)N(R11)R12, -C(0)N(R11)R12, -C(0) -N(R13)C(0)N(R11)R12, -N(R13)C(0)N(R11)S(0)2R43, -N(R10)C(0)N(R13)N(R11)R12, -N(R10)C(0)N(R13)N(R11)S(0)2R43, -N(R13)C(0)OR10, -P(0)OR10, or -P(0)(OR19)OR12. R4, R5, R6 and R7 = H, alkyl, alkenyl, alkynyl, aryl, heteroaryl, cycloalkyl, heterocyclyl, aralkyl, heteroaralkyl, -OR14, -SR14, -S(0)2R14, -N(R15)R16, -N(R15)S(0)2R43, -C(0)R18, -C(0)0R20, -C(0)N(R21)R22, -C(0)N(R21)S(0)2R43; -C(0)N(R42)N(R21)R22; or -C(0)N(R42)N(R21)S(0)2R43; or R4 and R5, or R4

and 86, or 84 and 87, or 85 and 86, or 85 and 87, or 86 and 87, together with the C atom to which they are attached, form a cyclealty, and and the heterocycly, or cyclealksny; ring, or together form a double born of the form and oxo, thiose, issues, oxides or a hydrazone, or 86 and 87, together with the C atom to which they are attached, form an exceyclic double bond, and 84 and 85 are as described above. 88 — alky, alknyl, alknyl, aryl, aryl, -c(C)0823, -(C)0821, 25. (C)08223, -(C)08223, -(C)082323, -(C)082333, -(C)08233, -(C)082333, -(C)0823333, -(

IT 629662-32-4P 629662-34-6P 629663-80-5P

629664-83-1P RI: PAC (Pharmacological activity); SFN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(drug candidate; preparation of azepinoindole and pyridoindole derivs as modulators of farnesoid X and/or orphan nuclear receptors)
8 52965-32-4 CAPLUS

CN 1H-Benzofuro[2,3-d]azepine-5-carboxylic acid,

3-(3,4-difluorobenzov1)-2,3-dihydro-, ethyl ester (CA INDEX NAME)

RN 629662-34-6 CAPLUS

CN 1H-[1]Benzothieno[2,3-d]azepine-5-carboxylic acid, 3-(3,4-difluorobenzovl)-2,3-dihydro-, ethyl ester (CA INDEX NAME)

RN 629663-80-5 CAPLUS

CN Spiro[azepino[4,5-b]indole-1(2H),2'-[1,3]dioxolane]-5-carboxylic acid, 3-(4-fluorobenzoyl)-3,6-dihydro-, ethyl ester (CA INDEX NAME)

RN 629664-83-1 CAPLUS

CN Spiro(azepino (4,5-b)indole-1(2H),1'-cyclopentane)-5-carboxylic acid,
3-(3,4-difluorobenzoyl)-3,6-dihydro-, ethyl ester (CA INDEX NAME)

IT 629662-33-5P 629664-84-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation of azepinoindole and pyridoindole derivs, as modulators of

(preparation of azepinoindole and pyridoindole derivs, as modulators of farnesoid X and/or orphan nuclear receptors) RN 629662-33-5 CAPLUS

CN 1H-Benzofuro[2,3-d]azepine-5-carboxylic acid, 2,3-dihydro-, ethyl ester (CA INDEX NAME)

RN 629664-84-2 CAPLUS

CN Spiro[azepino[4,5-b]indole-1(2H),1'-cyclopentane]-5-carboxylic acid, 3,6-dihydro-, ethyl ester (CA INDEX NAME) 10/565,702



OS.CITING REF COUNT:

REFERENCE COUNT:

- 9 THERE ARE 9 CAPLUS RECORDS THAT CITE THIS RECORD (9 CITINGS)
- 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L29 ANSWER 11 OF 27 CAPLUS COPYRIGHT 2011 ACS on STN

ACCESSION NUMBER: 2000:441796 CAPLUS

DOCUMENT NUMBER: 133:74016 TITLE: preparation of spirotricyclic compounds as H1 receptor

antagonists INVENTOR(S): Janssens, Frans Eduard; Leenaerts, Joseph Elisabeth

PATENT ASSIGNEE(S): Janssen Pharmaceutica N.V., Belg. SOURCE: PCT Int. Appl., 64 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANCHAGE: English

FAMILY ACC. NUM. COUNT: 1 PATENT INFORMATION:

PA:	TENT	NO.			KIND DATE			APPLICATION NO.						DATE						
WO							WO 1999-EP10176													
	W:	AE,	AL,	AM,	AT.	ΑU,	AZ.	BA,	BB,	BG	, BE	R.	BY.	CA,	CH.	CN,	CR.	CU,		
								FI,												
		IN,	IS,	JP,	KE,	KG,	KP,	KR,	KZ,	LC	, L	ĸ,	LR,	LS,	LT,	LU,	LV,	MA.		
								NO,										SI,		
		SK,	SL,	TJ,	TM,	TR,	TT,	TZ,	UA,	UG	, U.	s,	UZ,	VN,	YU,	ZA,	ZW			
	RW:																			
								IE,							SE,	BF,	BJ,	CF,		
			CI,	CM,	GA,	GN,	GW,	ML,	MR,	NE	, SI	N,	TD,	TG						
CA	2355	939			A1		2000	0629		CA	1999	9-2	355	939		1	9991	215		
CA	2355	939			C		2010	1214												
AU	2000	0304	12		A		2000	0712	- 1	ΑU	2000	0-3	041	2		19991215				
AU	7648.	20			B2		2003	0828												
BR	2355939 2000030412 764820 9916371				A		2001	0918	1	BR	1999	9-1	637	1		19991215				
EP	1144	411			A1		2001	1017	1	EΡ	1999	9-9	646	25		19991215				
EP	1144	411			B1		2005	0427		EP 1999-964625										
	R:							FR,	GB,	GF	, I	Γ,	LI,	LU,	NL,	SE,	MC,	PT,		
		IE,	SI,	LT,	LV,	FI,	RO													
TR	2001	0017	11		T2		2001	1221		TR	2001	1-1	711			1	9991	215		
HU	2001001711 2001004779 2001004779			A2		2002	0429	1	HU	2001	1-4	1779			19991215					
HU	2001	0047	79		A3		2003	1229												
EE	2001000328				A		20031229 E2 2001-328 20020015 E2 2001-328 20071015 U7 2005-58540 20071015 U7 2005-58540 20071015 U7 2005-58540 20071015 U7 2005-58540 2005-5854							1	9991	215				
EE	4917				B1		2007	1015												
JP	2002	5333	44		T		2002	1008		JΡ	2000	9-5	895	40		1	9991	215		
JP	4601	175			B2		2010	1222												
NZ	5128	70			A		2003	1128	1	NZ	1999	9-5	128	70		1	9991	215		
AT	2941	294178			T		2005	0515	- 1	AT 1999-964625							19991215			
PT	1144	1144411			E		2005	0930		PT 1999-964625							19991215			
ES	2242	443			Т3		2005	ES 1999-964625							19991215					
CN	1258	533			C.		2006	0607		CN	1999	9-8	147	05		1	9991	215		
PL	1962	62			В1		2007	1231		PL	1999	9-3	482	95		1	9991	215		
SK	2861	58			В6		2008	0407		SK	2001	1-8	314			1	9991	215		
TL	1437	6/			Α.		2010	0328		IЪ	1999	9-1	431	67		1	9991	215		
CZ	3019	53			B6		2010	0811		CZ	2001	1-2	2069			1	9991	215		
TW	250981			В	20060311				TW 1999-122194						1	9991	21/			
EG	24605			A		2010	0110		EG	1999	9-1	026			1	9991	400			
IN	2001	MNUU	991		Α.		2005	0304		ΙN	2001	1-6	sn44	I.		20010423				
IN	2120	18			A1		2008	0125		-	2001		0			-	0010	E O O		
BG DG	1055 6513 2001	40			A		2001	1231		DG	2001	1-1	055	40		2	0010	529		
BG	0013	3	1.0		81		2007	0.530		w.	2001		210			2	0010	C01		
140	Z001	0027	10		A		2001	0.001		INO.	2001	1-2	110			- 2	0010	100		

PR1

NO 318891	B1	20050518				
HR 2001000453	A2	20020630	HR	2001-453		20010615
HR 2001000453	B1	20100731				
MX 2001006244	A	20010910	MX	2001-6244		20010618
ZA 2001004977	A	20020618	ZA.	2001-4977		20010618
US 7148214	B1	20061212	US	2001-868535		20010726
HK 1043128	A1	20070119	HK	2002-104999		20020703
US 20050026901	A1	20050203	US	2004-898844		20040726
US 7087595	B2	20060808				
IORITY APPLN. INFO.:			EP	1998-204347	A	19981219
			WO	1999-EP10176	W	19991215
			TTC	2001-060535	3.1	20010726

ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT OTHER SOURCE(S): MARPAT 133:74016

AB Title compds. [I; R = 222385, 22880085, 2285; R1 = B, halo, alkyl, acyl, etc.; R2 = B, halo, alkyl, aryl, etc.; R3R4 = YGH:GI, BCHGT, GH:GHGT:GR, S5 = (un)substituted heteroaryl, -tct.haydrofuranyl, etc.; Y = O, S, (alkyl):mino, alkanoylimino; Z = alkylene, GH:GM, GH:GM, GH:GM, CH:GM, CH:GM,

1-phenylmethyl:-H=inidazole was condensed with 1-phenylmethyl--piperidone and the produced only on stern phylogenetics, [RI = R2 = H, R3R4 = CH:CHGH:CH, Z = CH2, Z1 = CH2CH2) [H1; R = H) which was N=alkylated by 1-(2-phenothyl)-4-ethyl-1,4-dhilydro-2Hettaraol-5-one to give II [R = Z-(4-chyl-5-coxo-1,4-chilydro-1H-tetrazol-1-yl)ethyl]. Data for biol. activity of 1 services of the condition of th

IT 279253-82-6P

RJ: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SFN (Synthetic preparation); TBU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of spirotricyclic compds. as H1 receptor antagonists) RN 279253-82-6 CAPLUS

CN Spiro[cyclohexane-1,10*-[10H]imidazo[1,2-a]thieno[3,2-d]azepine], (2E)-2-butenedioate (1:1) (CA INDEX NAME)

CM 1 CRN 279253-81-5 CMF C15 B16 N2 S

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

10/565,702

CM 2

CRN 110-17-8

CMF C4 H4 O4

Double bond geometry as shown.

HO2C E CO2H

OS.CITING REF COUNT: 5

- THERE ARE 5 CAPLUS RECORDS THAT CITE THIS RECORD (7 CITINGS)
- REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L29 ANSWER 12 OF 27 CAPLUS COPYRIGHT 2011 ACS on STN

ACCESSION NUMBER: 1998:203750 CAPLUS DOCUMENT NUMBER: 128:282795

ORIGINAL REFERENCE NO.: 128:55983a,55986a TITLE:

Synthesis of pyrrolidinothieno-(or [1]benzothieno)[3]azepinones from the corresponding

п

azepinediones or N-(thienvl or [1]benzothienv])acetylprolinals

AUTHOR(S): Othman, Mohamed; Netchitailo, Pierre; Decroix, Bernard Lab. Chimie, Fac. Scis. Techniques, Univ. Havre, Le

Havre, 76600, Fr. SOURCE . Heterocycles (1998), 48(2), 335-346

CODEN: HTCYAM; ISSN: 0385-5414 PUBLISHER: Japan Institute of Heterocyclic Chemistry

DOCUMENT TYPE: Journal LANGUAGE: English



R1CH=CHRCH2CON ORC

Title compds. I [RR] = CH:CHS, SCH:CH, o-C6H4S, o-SC6H4] were prepared from AB the diones or by direct cyclization of prolinals II.

205761-43-9P 205761-47-3P RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of pyrrolidinothienoazepinones) 205761-43-9 CAPLUS RN

5H-Pyrrolo[1,2-a]thieno[2,3-d]azepin-5-one, 4,7,8,9-tetrahydro- (CA INDEX CN NAME)



RN 205761-47-3 CAPLUS

CN 5H-[1]Benzothieno[2,3-d]pyrrolo[1,2-a]azepin-5-one, 1,2,3,6-tetrahydro-

(CA INDEX NAME)



OS.CITING REF COUNT: REFERENCE COUNT:

- 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD (1 CITINGS)
- 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L29 ANSWER 13 OF 27 CAPLUS COPYRIGHT 2011 ACS on STN

ACCESSION NUMBER: 1997:140708 CAPLUS DOCUMENT NUMBER: 126:131678

ORIGINAL REFERENCE NO.: 126:25437a,25440a
TITLE: Flow Thermolysis Rearrangements in the Indole Alkaloid

Series: Strictamine and Akuammicine Derivatives. The Absolute Configurations of Ngouniensine and eni-Ngouniensine

AUTHOR(S): Hugel, Georgette; Royer, Daniel; Le Men-Olivier, Louisette; Richard, Bernard; Jacquier, Marie-Jose;

Levy, Jean
CORPORATE SOURCE: Laboratoire de Transformations et Synthese de

Substances Naturelles et Laboratoire de

Pharmacognosie, Universite de Reims Champagne-Ardenne Faculte de Pharmacie, Reims, F-51096, Fr. SOURCE: Journal of Organic Chemistry (1997), 62(3), 578-583

SOURCE: JOINTAI OF ORGANIC CHEMISTRY (
CODEN: JOCEAH; ISSN: 0022-3263
PHRLISHER: American Chemical Society

PUBLISHER: American Chemical Society DOCUMENT TYPE: Journal

LANGUAGE: English
OTHER SOURCE(S): CASREACT 126:131678

AB Flow thermolysis of strictanine generated two of the predictable rearrangement products, resulting from [1,5]-signatropic shifts: akuammicine and indolenine I. Besides formation of these two compds., a quite different pathway gave rise to a novel rearrangement leading to a Rearrangement bed to the approximation of the second shifts of the s

RL: SPN (Synthetic preparation); PREP (Preparation)
(flow thermolysis rearrangements of indole alkaloids strictamine and
akuammicine derivs., absolute configurations of naouniensine and

epi-ngouniensine) RN 186252-97-1 CAPLUS

CN 5H-Pyrido[1',2':1,2]azepino[4,5-b]indole-6-carboxaldehyde, 9-ethyl-9,10,12,13-tetrahydro-, (9S)- (CA INDEX NAME)

Absolute stereochemistry.



OS.CITING REF COUNT:

- THERE ARE 6 CAPLUS RECORDS THAT CITE THIS RECORD (7 CITINGS)
- REFERENCE COUNT: 30 THERE ARE 30 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L29 ANSWER 14 OF 27 CAPLUS COPYRIGHT 2011 ACS on STN

ACCESSION NUMBER: 1995:419668 CAPLUS DOCUMENT NUMBER: 122:265125

ORIGINAL REFERENCE NO.: 122:48400h, 48401a

TITLE: Synthesis of biliverding with stable extended

conformations. Part II

AUTHOR(S): Bari, Sara E.; Iturraspe, Jose; Frydman, Benjamin

CORPORATE SOURCE: Fac. Farm. Bioquim., Univ. Buenos Aires, Buenos Aires,

SOURCE: Tetrahedron (1995), 51(8), 2255-66

CODEN: TETRAB; ISSN: 0040-4020

PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English

OTHER SOURCE(S): CASREACT 122:265125

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

- AB The synthesis of two hexacyclic, I and II, and one heptacyclic biliverdin, III, with extended contractions was achieved using base catalyzed. III, with extended contractions are achieved using base catalyzed by 2-chlorosthy! residues were located at selected pryrrole positions as to enable them to react with proximal basic introgens at the adjacent pyrrole rings. Seven membered rings were than formed which distorted members are actively as the seven and the seven as the seven as a seven
 - backbone can achieve.

 T 118631-58-6P 130877-88-2P 162661-71-4P
 RL: SPN (Synthetic preparation); FREP (Preparation)
 (synthesis of hexacyclic and heptacyclic biliverdins)
- RN 118631-58-6 CAPLUS

CN Dipyrrolo[1,2-a;2',3'-d]azepine-9-propancic acid, 2-[4,5-dihydro-9'-3-methowy-3-oxopropyl)-3,8-dimethyl-7-oxodipyrrolo[1,2-a;2',3'-d]azepin-2(7H)-ylidene]methyl]-1,4,5,7-tetrahydro-3,8-dimethyl-7-oxo-, methyl ester, (2)- (SCI) (CAINDER NAME)

Double bond geometry as shown.

RN 130877-88-2 CAPLUS
CN Pyrrolo[1-2-a]pyrolo[1"",2"":1"",7" | azepino[4"",5"":4",5"]pyrrolo[1-2-a]pyrolo[1",2":1",7" | azepino[4",5":4,5]pyrrolo[2,3-d]azepino-2,12-dipropanoic acid, 3,5,6,7,8,13,15,16-octahydro-1,11,17-trimethyl-3,13-dioxo-, 2.12-dimethyl ester (CA INDEX NAME)

PAGE 1-B

— оме

RN 162661-71-4 CAPLUS

CN 10H-Dipyrrolo[1*,2*-a*:2,3-d]pyrrolo[1,5-a:2,3-d*]bisazepine-9-propanoic acid, 2-[1,5-d*]hydro-4-(3-nethoxy-3-oxoproyl)-3-enthyl-5-oxo-2H-pyrrol-2ylidene]nethyl]-4,5,12,13-tetrahydro-3,8,14-trinethyl-10-oxo-, methyl ester. (2)- (9C1) (CR.INEEN.NME)

Double bond geometry as shown.

PAGE 1-A

PAGE 1-B

OS.CITING REF COUNT: 5 THERE ARE 5 CAPLUS RECORDS THAT CITE THIS RECORD (5 CITINGS)

L29 ANSWER 15 OF 27 CAPLUS COPYRIGHT 2011 ACS on STN

ACCESSION NUMBER: 1995:419667 CAPLUS DOCUMENT NUMBER: 122:290543

ORIGINAL REFERENCE NO.: 122:52971a,52974a
TITLE: Synthesis of biliverdins with stable extended

conformations. Part I
AUTHOR(S): Iturraspe, Jose; Bari, Sara E.;

AUTHOR(S): Iturraspe, Jose; Bari, Sara E.; Frydman, Benjamin CORPORATE SOURCE: Fac. Farm. Bioquimica, Univ. Buenos Aires, Buenos Aires, 1113, Argent.

SOURCE: Tetrahedron (1995), 51(8), 2243-54

CODEN: TETRAB; ISSN: 0040-4020 PUBLISHER: Elsevier

DOCUMENT TYPE: Journal LANGUAGE: English

OTHER SOURCE(S): CASREACT 122:290543
AB Biliverdins with extended conformations stabilized by intramol. Et bridges

were obtained by hase treatment of helical biliverdins with 2-chloroethyl side chains. Thus, mobilitywordin [5] was obtained by reaction of 13,18-df(2-chloroethyl)-biliverdin with DEB. During the reaction, the 2-chloroethyl-f(3) resides underwent an intramel. substitution reaction with N-24 while the 2-chloroethyl-C[8] residue underwent an elimination reaction from a winyl residue. This reaction scheep was unambiguously

demonstrated by performing the synthesis of [158-24]-dihydro-mobiliverdin IRB and of [158-23]-dihydrophorcabilin. The method was then applied to the synthesis of mobiliverdin IRG, a natural product isolated when the 2-chlorocethy; side chains are at C(3) (or the equivalent C(17)) and C(2) (or the equivalent C(18)) positions of the biliverdin, elimination reactions lead to vinyl residues in basic sedies at any other of the

β-pyrrole sites, treatment with base leads to the formation of seven-membered rings by intramol. substitution reactions.

T 118631-57-5P 163014-57-1P
RN: SPN (Synthetic preparation); PREP (Preparation)
(synthesis of pentacyclic biliverdins)

(synthesis of pe RN 118631-57-5 CAPLUS

CN IH-Pyrrole-3-propanoic acid, 2-[[2-[[8-ethenyl-1,4,5,7-tetrahydro-3,9-disethyl-7-oxodityrolo][2,-3-2]]methylenel-4(3-methoxy-3-oxopropyl)-3-methyl-2H-pyrrol-5-yl]methylene]-2,5-dihydro-4-methyl-5-oxopmethyl-ether, (2,2) [9CI] (CA INDEX NBME)

Double bond geometry as shown.

RN 163014-57-1 CAPLUS

CN III-Pyrrole-3-propanoic acid, 2-[12-1(6-ethyl-1,4,5,7-tetrahydro-3,9-disethyl-7-oxodipyrolol], 2-a:2-3, 3-diazehyl-3-y-6-13) methylone] -4-(3-methoxy-3-oxopropyl)-3-methyl-2ll-pyrrol-5-yl]sethylene]-2,5-dihydro-4-methyl-5-oxo-, methyl ester, (Z, Z, 1) (2CI) (CA INDEX NMEX)

Double bond geometry as shown.

OS.CITING REF COUNT: 6 THERE ARE 6 CAPLUS RECORDS THAT CITE THIS RECORD (6 CITINGS)

L29 ANSWER 16 OF 27 CAPLUS COPYRIGHT 2011 ACS on STN

ACCESSION NUMBER: 1994:605360 CAPLUS DOCUMENT NUMBER: 121:205360

ORIGINAL REFERENCE NO.: 121:37397a,37400a
TITLE: Preparation of antiallergic triazolo(pyrrolo, thieno

or furano) azepine derivatives
INVENTOR(S): Janssens, Frans Eduard: Lacrampe, Jean Fernand Armand;

PATENT ASSIGNEE(S): Pantage Pharmaceutica N.V., Belg.

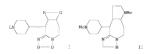
SOURCE: PCT Int. Appl., 42 pp.

CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1 PATENT INFORMATION:

PA	PATENT NO.						KIND DATE			APPLICATION NO.							DATE		
WO	9413681			A1 19940623			WO 1993-EP3322							19931125					
	W:						CZ,						KR,	LK,	LV,	MG,	MN,	MW.	
							SD,												
	RW:																		
		BF,	BJ,	CF,	CG,	CI,	CM,	GA,	GN,	MI	., h	Æ,	NE,	SN,	TD,	TG			
CA	A 2150804			A1 19940623				CA 1993-2150804 AU 1994-56280							19931125				
CA	2150	304			C		2006	1010											
AU	94562	280			A		1994	0704	- 1	ΑU	199	94-5	628	0		1	9931	125	
AU	6767	03			B2		1997	0320											
EP	6758	39			A1		1995	1011	1	EΡ	199	94-9	9018	88		1	9931	125	
EP	67581	39			B1		2000	0705											
	R:	AT,	BE,	CH,	DE,	DK,	ES,	FR,	GB,	GF	3, 3	Œ,	IT,	LI,	LU,	NL,	PT,	SE	
HU	7180 2234 0850 3503	3			A2		1996	0228		HU	199	95-1	1619			1	9931	.125	
HU	2234	55			B1		2004	0728											
JP	08503	3954			T		1996	0430		JΡ	199	94-5	5137	22		1	9931	125	
JP	3503	065			B2		2004	0302											
RU	2127 1765 1943 2149	737			C1		1999	0320	1	RU	199	95-1	1155	15		1	9931	.125	
PL	17652	28			B1		1999	0630		PΕ	199	93-3	3092	55		1	9931	125	
AT	1943	50			T		2000	0715	- 1	AT	199	94-9	9018	88		1	9931	125	
ES	2149	361			Т3		2000	1116	1	ES	199	94-9	9018	88		1	9931	125	
PT	6758	39			E		2000	1229		PT	199	34-1	9018	88		1	9931	125	
US	5595	988			A		1997	0121	1	US	199	95-4	1333	87		1	9950	508	
FI	9502	724			A		1995	0602		PI	199	95-2	2724			1	9950	602	
NO	95022	200			A		1995	0803	1	NO	199	95-2	2200			1	9950	602	
NO	3116	19			B1		2001	1217											
GR	3034	195			Т3		2000	1229		GR	200	00-	1021	84		2	0000	928	
PRIORIT	9502: 3116: 3034: Y APPI	LN.	INFO	. :					1	EΡ	199	92-2	2037	77		A 1	9921	204	
									1	EΡ	199	94-9	9018	88		A 1	9931	125	
									1									125	

ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT OTHER SOURCE(S): MARPAT 121:205360



AB Title compds. I (E-G = XCRICH, GH:CRZX wherein X = Q, S or R3M wherein R3 = H; Cl-6 alkyl, Cl-4 alkyl, alkyloarbonyl, R1, R2 = H; Cl-6 alkyl, blad, (substituted) ethenyl, etc.; B0 = CR4:N, N:CRS wherein R4 H; Cl-4 alkyl, cubstituted) ethenyl, mo-Cl-4 alkyl, BCO, B0CC, R5 = H, Rh, pyrdinyl, etc.; L = H, (substituted) Cl-6 alkyl, (aryl) Cl-6 alkenyl, Alk-Y-Bet, Alk-R1C-H, Cl-4 alkenyl, Y = Q. S, RH, Bet = (substituted) heterocyclyl) or a salt or steromer thereof, are prepared (1-Mctuty-1-piperidnyl) III-[2-(1-Mctuty-1-Bryerio-2-y)] ethyl - His! 1.2, 2.4 (substituted) heterocyclyl) or a salt or steromer thereof, are prepared (1-Mctuty-1-piperidnyl) III-[2-(1-Mctuty-1-Bryerio-2-y)] ethyl - His! 1.2, 2.4 (substituted) heterocyclyl).

IT 1236831-63-2

RL: PRPH (Prophetic) (Preparation of antiallergic triazolo(pyrrolo, thieno or furano) azepine derivatives)

RN 1236831-63-2 CAPLUS

CN INDEX NAME NOT YET ASSIGNED



IT 158144-23-1P 158144-25-3P 158144-26-4P RL: RCT (Reactant): SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and reaction of, in preparation of antiallergy agents) RN 158144-23-1 CAPLUS

CN 10H-Thieno[3,2-d]-1,2,4-triazolo[4,3-a]azepine (CA INDEX NAME)



RN 158144-25-3 CAPLUS CN 10H-Thieno[3,2-d][1,2,4]triazolo[1,5-a]azepin-10-one (CA INDEX NAME)

RN 158144-26-4 CAPLUS CN 10H-Thieno[3,2-4][1,2,4]triazolo[1,5-a]azepin-10-ol, 10-(1-methyl-4-piperidinyl)- (CA INDEX NAME)

IT 158143-86-3P 158143-89-6P 158144-02-6P 158144-10-6P RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of, as antialleroy agent)

RN 158143-86-3 CAPLUS CN 10H-Thieno(3,2-d)-1,2,4-triazolo[4,3-a]azepine, 10-(1-methyl-4-piperidinylidene)- (CA INDEX NAME)

158143-89-6 CAPLUS

CN Pyrrolo[3,2-d][1,2,4]triazolo[1,5-a]azepine,
7,10-dihydro-10-[1-[2-(4-methoxyphenyl)ethyl]-4-piperidinyl]-7-methyl-(CA INDEX NAME)

RN 158144-02-6 CAPLUS CN

10H-Furo[3,2-d][1,2,4]triazolo[1,5-a]azepine, 8-methyl-10-(1-methyl-4-piperidinyl)- (CA INDEX NAME)

- RN 158144-10-6 CAPLUS
- CN 1-Piperidinepropanoic acid, 4-(10H-thieno[3,2-d]-1,2,4-triazolo[4,3-a]azepin-10-ylidene)-, methyl ester (CA INDEX NAME)

- CH2-CH2-C-OMe
- OS.CITING REF COUNT:
- THERE ARE 5 CAPLUS RECORDS THAT CITE THIS RECORD (5 CITINGS)
- REFERENCE COUNT:
- THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L29 ANSWER 17 OF 27 CAPLUS COPYRIGHT 2011 ACS on STN

ACCESSION NUMBER: 1993:213072 CAPLUS

DOCUMENT NUMBER: 118:213072 ORIGINAL REFERENCE NO.: 118:36731a,36734a

TITLE: Proparation of imidazo[1,2-a](pyrrolo, thieno or furano) [3,2-d] azepines as allergy inhibitors
INVENTOR(S): Janusens, Frans Eduard; Diels, Gaston Stanizlas
Marcella; Leenaertz, Joseph Elizabeth; Cooymans,

PATENT ASSIGNEE(S): Janssen Pharmaceutica N.V., Belg.

SOURCE: Eur. Pat. Appl., 60 pp.

DOCUMENT TYPE: Patent

LANGUAGE: English FAMILY ACC. NUM. COUNT: 1 PATENT INFORMATION:

PATENT NO.							D	DATE	ATE			PLIC	AT I	DATE							
	ED 510404							10001016			EP 1992-201665							10000000			
		R:	PT																		
	IL 101851				A 19960514					IL	1992	19920513									
	CN 1068116				A		19930120			IL 1992-101851 CN 1992-104830							19920516				
	CN 1033587				C		19961218														
	CA 2102889 CA 2102889				A1 19921214				CA	1992	19920609										
	CA 2102889				C 20021126																
	WO 9222553					A1		19921223			WO 1992-EP1331						19920609				
		W:					CA,	CS,	FI,	HΨ,	J.	, K	?,	KR,	LK,	MG,	MW,	NO,	PL,		
				RU,																	
		RW:														FR,	GΑ,	GB,	GN,		
			GR,	IT,	LU,	MC,	ML,	MR,	NL,	SE,	SI	, T	٠,	TG							
	AU	9219011				A.	19930112			AU 1992-19011							19920609				
	AU	652841				B2		19940908													
	EP	5888 5888	59			A1		1994	0330		EP	199	2-9	116	93		1	9920	609		
		R:																			
	JP	0650 3182	7890			T		1994	0908		JP	199	2-5	107.	34		1	9920	609		
	JP	3182	421			B2		2001	0703												
	HU	7042	В			A2		1995	1030		HU	199	3-3	3554			1	9920	609		
	HU	7042 2210 1703	13			BI		2002	0729												
	ЬP	2471	/6			BI		1996	0815		PЬ	199	2-3	MTR.	19		- 1	9920	609		
	AT	24/1	18			T		2003	0812		AT	199	2-9	3116	13		1	9920	609		
	ES	2204 9204 5461	892			T3		2004	0501		ES	199	2-9	116	43		1	9920	609		
	ZA	9204	321			A		1993	1213		ZA.	199		1321			- 1	9920	P12		
	US	5461	050			A		1995	1024		US	199.	5-1	1201	21		1	9931	129		
	NO	9304 3006	493			A		1994	0104		NO	199.	5-4	1493			1	9931	209		
	NO	3006	89			BI		1997	0/0/												
PRIORITY APPLA. INFO.:					BI		1333		FI 1993-5557 US 1991-714487						19931210						
PRIOR	TT:	MPP.	LIN.	INFO	. :													9910 9920			

ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT

OTHER SOURCE(S): MARPAT 118:213072

GI For diagram(s), see printed CA Issue.
Ba Title compds. [Ir RI = H, alkyl, halo, ethenyl substituted with CO2H or alkoxycarbonyl, hydroxylaikyi, CHO, BO2C, hydroxycarbonylaikyi; R2 = H, alkyl, ethenyl or alkyl substituted with CO2H or alkoxy carbonyl,

hydroxyalkyl, CHO, CO2H; R3 - H, alkyl, hydroxyalkyl, Ph, halo; L - H,

(substituted) alkyl, alkenyl, ZYQl, ZNHCOQ2, ZQ37 Y = 0, S, NH; Z = Cl-4 alkylene; Ql, Q2 = (austituted) furyl, thienyl, oxazolyl, thiazolyl, imidazolyl, pyrralyl, pyrazolyl, thiadlarolyl, oxodiazolyl, pyriadinyl, pyrazolyl, jimidazolyl, $\Delta = (pridar_2 - y_1 r_3 - q_1)$, (austituted)

4,5-dihydro-5-oxo-1H-tetrazolyl, 2-oxo-3-oxazolidinyl, 2-oxo-3-oxazolidinyl, 2,3-dihydro-2-oxo-1H-bonzimidazol-1-yl, etc.; X - O, S, NR5; R5 - H, alkyl, alkoxycarrbonyl; dotted lines = optional double bonds] were prepared as broad spectrum antiallergics with oxcellent oral availability, lack of

sedating properties, fast easet of action, and favorable duration of action (no data). Thus, [2-fl-sethyl-il-lpyprol-2-yl-lethyl] methanesul fonate was refluxed 3 daysa with inidazole and K203 in THF to give 61.78 1-[2-(1-sethyl-il-Hpyprol-2-yl-lethyl]-IH-indazole. The later and then Et6 1-methyl-4-piperidinearboxylate were added to a -70° mixture of (WGJD)ZNNI and Ball in THF. The mixture was stirred 1 h at

-70° and 2 h at room temperature ti give 60% (1-methyl-4-piperidinyl)[1-[2-(1-methyl-1H-pyrrol-2-yl]ethyl]-1H-imidazol-2-yl]methanone. This was stirred with MeSO3H at 80° to give 10.8%

title compound II. Pharmaceutical I formulations are given.
I1 146800-71-7P 146800-72-8P 147184-18-1P 147184-19-8P 147184-20-1P 147184-22-3P 147184-24-5P 147184-27-8P 147210-29-55P

RI: BAC [Biological activity or effector, except adverse); BSU (Biological study, unclassified); SFN (Synthetic preparation); RBU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation of, as allerow inhibitor)

RN 146800-71-7 CAPLUS CN 10H-Imidazo[1,2-a]thieno[3,2-d]azepine, 10-(1-methyl-4-piperidinyl)- (CA TNDEX NAME)

RN 146800-72-8 CAPLUS

CN 10H-Imidazo[1,2-a]thieno[3,2-d]azepine, 10-(4-piperidinylidene)- (CA INDEX NAME)

RN 147184-18-7 CAPLUS CN 10H-Imidazo[1,2-a]thieno[3,2-d]azepine, 10-(1-methyl-4-piperidinylidene)-(CA INDEX NAME)



RN 147184-19-8 CAPLUS CN Imidazo[1,2-a]pyrrolo

Imidazo[1,2-a]pyrrolo[3,2-d]azepine,
7,10-dihydro-7-methyl-10-(1-methyl-4-piperidinyl)- (CA INDEX NAME)



RN 147184-20-1 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-(108-imidazo[1,2-a]thieno[3,2-d]azepin-10-ylidene)-, ethyl ester (CA INDEX NAME)

- RN 147184-22-3 CAPLUS CN 10H-Imidazo[1,2-a]thieno[3,2-d]azepine, 10-(4-piperidinylidene)-, hydrochloride (1:1) (CA INDEX NAME)
- S N
 - HCl

CM 1

- RN 147184-24-5 CAPLUS
 CN 10H-Imidazo[1,2-a]thieno[3,2-d]azepine,
 10-[1-[2-(4-methoxymbenyl)ethyl]-4-niperid;
 - 10-[1-[2-(4-methoxyphenyl)ethyl]-4-piperidinylidene]-, ethanedioate (2:5) (CA INDEX NAME)
 - CRN 147184-23-4 CMF C24 H25 N3 O S

CM 2

CRN 144-62-7 CMF C2 H2 O4

0 0 0-с-с-он

RN 147184-27-8 CAPLUS

CN 10H-Imidazo[1,2-a]thieno[3,2-d]azepine, 10-(1-methyl-4-piperidinyl)-, hydrochloride (1:2) (CA INDEX NAME)

●2 HC1

147210-29-5 CAPLUS

5H-Thiazolo[3,2-a]pyrimidin-5-one,

RN

CN

```
CM 1

GRN 147210-28-4

CMF C24 H23 N5 O S2

S

LH2

H0

CH2
```

6-[2-[4-(10H-imidazo[1,2-a]thieno[3,2-d]azepin-10-ylidene)-1piperidinyl[ethyl]-7-methyl-, ethanedioate (1:2) (CA INDEX NAME)

HO-C-C-OH

CM 2 CRN 144-62-7 CMF C2 H2 O4

IT 146800-88-6P, 4H-Thieno[2,3-d]azepin-5-amine
146800-89-7P 146800-90-0P,
10H-Imidazo[1,2-a]thieno[3,2-d]azepine 146800-91-1P
146800-92-2P
RL SPN (Synthetic preparation); PREP (Preparation)

(preparation) (preparation) FREE (Preparation)
(preparation of, as intermediates for imidazolazoloazepine inhibitor)
RN 146800-88-6 CAPLUS

CN 4H-Thieno[2,3-d]azepin-5-amine (CA INDEX NAME)

RN 146800-89-7 CAPLUS

N 4H-Thieno[2,3-d]azepin-5-amine, N-(2,2-dimethoxyethyl)- (CA INDEX NAME)

OMe

MeO-CH-CH₂-NH

CN 10H-Imidazo[1,2-a]thieno[3,2-d]azepine (CA INDEX NAME)

RN 146800-91-1 CAPLUS

CN 10H-Imidazo[1,2-a]thieno[3,2-d]azepin-10-one (CA INDEX NAME)

RN 146800-92-2 CAPLUS

CN 10H-Imidazo[1,2-a]thieno[3,2-d]azepin-10-o1, 10-(1-methyl-4-piperidinyl)-(CA INDEX NAME)



OS.CITING REF COUNT: 7 THERE ARE 7 CAPLUS RECORDS THAT CITE THIS RECORD (7 CITINGS)

L29 ANSWER 18 OF 27 CAPLUS COPYRIGHT 2011 ACS on STN

ACCESSION NUMBER: 1993:34948 CAPLUS DOCUMENT NUMBER: 118:34948

ORIGINAL REFERENCE NO.: 118:6287a,6290a
TITLE: The interplay between basicity, conformation, and

enzymic reduction in biliverdins
AUTHOR(S): Bari, Sara; Frydman, Rosalia B.; Grosman, Claudio;
Frydman, Benjamin

CORPORATE SOURCE: Fac. Farm. Bioquim., Univ. Buenos Aires, Buenos Aires, Argent.

SOURCE: Biochemical and Biophysical Research Communications

(1992), 188(1), 48-56 CODEN: BBRCA9; ISSN: 0006-291X

DOCUMENT TYPE: Journal LANGUAGE: English

AB Biliverdins with extended conformations are reduced by biliverdin reductase (BvR) at higher rates than biliverdins with helical

remarkably lower at import later than biliverians with merical conformations. To find out the mol. basis for this important feature of BVR mechanism, helical and extended biliverdins were titrated for their acid-base equilibrium in a protic solvent (methanol). The basicity of biliverdins increased with the stretching of the conformation. Biliverdin $IX \gamma$ (all-sym) has a pKa = 3.6; 5.10, 15.9, 5.9

a pKa = 3.7; 5,10,15-syn,anti,syn-biliverdin has a pKa = 6.1; 5,10,15-syn,anti,anti-biliverdin has a pKa = 6.4; and

5,10,15-all-anti-biliverdin has a pKs — 7.9. The increase in basicity with progressive stretching of conformations closely parallels the increase in the reduction rates by BWR. A biliverdin constrained by a 4-carbon chain to a helical conformation and which is a very weak base (pKs — 0.4) is not reduced by BWR. Nucleophilic addns. of —amcraptochanic at the Clo in biliverdine closely parallel their

Z-mercaptoethanol at the CIO in biliverding closely parallel their basicities, as can be expected if the formation of a pos. mesomeric species at CIO is linked to the basicity (i.e., the ease of protonation) 130877-88-2 14598-48-1 ering.

RL: RCT (Reactant); RACT (Reactant or reagent)

(reaction of, with biliverdin reductase, substrate conformation and basicity in relation to)

RN 130877-88-2 CAPLIS
CN Pyrrolo[1,2-a]pyrrolo[1***,2***:1***,7***]azepino[4***,5***:4**,5***]pyrrolo[1,2-a]pyrrolo[1,2-a]pyrrolo[2,3-d]azepine-2,12-dipropancic acid, 3,5,6,7,8,13,15,16-octahydro-1,11,17-trimethyl-3,13-dioxo-,2,12-dienthyl ester (CA INDEX NAME).

PAGE 1-B

- oMe

RN 145089-48-1 CAPLUS

N 101-Dipyrrolo(1*,2**-a*12,3-d]pyrrolo(1;5-a*2,3-d*1)bisazopine-8-propanoic acid, 2-(1,5-di)hydro-4-(3-asthoxy-3-oxoproy);1-3-asth)-4-oxo-28-pyrol-2-yi idene | asthyl | 3-d,5:12,13-tetrahydro-3,8,14-trinethyl-10-oxo-, methyl ester (9Cl) (CA INEX NAME).

PAGE 1-A

PAGE 1-B

- OMe

OS.CITING REF COUNT: 4 THERE ARE 4 CAP

4 THERE ARE 4 CAPLUS RECORDS THAT CITE THIS RECORD (4 CITINGS)

L29 ANSWER 19 OF 27 CAPLUS COPYRIGHT 2011 ACS on STN

ACCESSION NUMBER: 1992:526659 CAPLUS DOCUMENT NUMBER: 117:126659

ORIGINAL REFERENCE NO.: 117:21869a,21872a
TITLE: Reconstitution of apomyoglobin with extended

ITLE: Reconstitution biliverding

AUTHOR(S): Fernandez, Marcelo; Frydman, Rosalia B.; Bari, Sara;
Frydman, Benjamin

CORPORATE SOURCE: Fac. Farm. Bioquim., Univ. Buenos Aires, Buenos Aires,

SOURCE: Biochemical and Biophysical Research Communications

(1992), 183(3), 1209-15 CODEN: BBRCA9: ISSN: 0006-291X

DOCUMENT TYPE: Journal LANGUAGE: English

AB An anal. of the reconstitution of biliverdins with extended conformations and horse heart apomyoglobin was carried out. Biliverdins with the

52-syn, 102-syn, 152-anti and 52-anti, 102-syn, 152-anti conformations, as well as biliverdins with the 2,2,2 all-syn conformation recombined with appropriate. In every case the P enantiomers were bound in excess to the M enantiomers, with the exception of the 5-syn, 10-syn, 15-anti biliverdins where the M enantiomer bound preferentially to the protein.

Diliverding where the M emantioner bound preferentially to the protein.

Billiverding with an anti conformation at the C-10 meso bridge did not recombine with the protein. It was concluded that the presence of a syn conformation at the C-10 methine conformation between the conformation at the C-10 methine conformation process. This regions electivity to fit into the apomyoglobin heme procest. This regions electivity of the heme procket is of importance in view of the well-known analogy

between the ligand domains of myoglobin and the C-phycocyanins. 130877-84-8 143222-57-5 143222-59-7 RL: PRP (Properties)

(apomyoglobin reconstitution with, structure in relation to) N 130877-84-8 CAPLUS

ON Pyrcolo[1,2-a pyrcolo[1] , 2-11,1 , 711 | axepino[4",5",4",5") pyrcolo[1,2-a] pyrcolo[1] , 2-11,2 pyrcolo[1,2-d] axepino[4,5] , 4,5 pyrcolo[2,3-d] axepino[4,2-d] pyrcolo[2,3-d] axepino[4,2-d] pyrcolo[2,3-d] axepino[4,2-d] , 15,16-octahydro-1,11,17-trimethyl-3,13-dioxo-(CA INDEX MAME)

RN 143222-57-5 CAPLUS

CN Dipyrrolo[1,2-a:2',3'-d]azepine-9-propanoic acid,

2-[[9-(2-carboxyethy]]-4,5-dihydro-3,8-dimethyl-7-oxodipyrrolo[],2-a:2',3'-d]azepin-2(7H)-ylidene]methyl]-1,4,5,7-tetrahydro-3,8-dimethyl-7-oxo-,(Z)-(9CI) (CAINDEX NAME)

Double bond geometry as shown.

PAGE 1-A NΕ HO₂C

PAGE 1-B

~ co2H

RN

143222-59-7 CAPLUS 5H-Dipyrrolo[1,5-a:2,3-d']bisazepine-9-propanoic CN acid, 2-[[4-(2-carboxyethyl)-1,5-dihydro-3-methyl-5-oxo-2H-pyrrol-2ylidene]methyl]-4,10,12,13-tetrahydro-3,8,14-trimethyl-10-oxo-, (Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

PAGE 1-B

- CO2H

OS.CITING REF COUNT: THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD (1 CITINGS)

L29 ANSWER 20 OF 27 CAPLUS COPYRIGHT 2011 ACS on STN

ACCESSION NUMBER: 1991:2582 CAPLUS
DOCUMENT NUMBER: 114:2582

ORIGINAL REFERENCE NO.: 114:531a,534a

TITLE: The enzymic and chemical reduction of extended

biliverdins

AUTHOR(S): Frydman, Rosalia B.; Bari, Sara; Tomaro, Maria L.;
Frydman, Benjamin
COPPORATE SOURCE: Pac. Parm. Bioquim. Heiv. Buenes Aires, Buenes Air

CORPORATE SOURCE: Fac. Farm. Bioquim., Univ. Buenos Aires, Buenos Aires, Argent.
SOURCE: Biochemical and Biophysical Research Communications

(1990), 171(1), 465-73 CODEN: BBRCA9; ISSN: 0006-291X

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The substrate specificity of rat liver biliverdin reductase was probed using helical and extended biliverdins. The former were the ZZZ-all-syn

biliverdins IX a and IX y, and the latter were the 5%-sym, 10E-anti, 15Z-sym; 10Z-sym, 15Z-anti, 15Z-sym; 10Z-sym, 15Z-sym, 10E-anti, 15Z-sym; 10Z-sym, 10E-anti, 10Z-sym, 10Z-sym, 10E-anti, 10Z-sym, 10Z-sym, 10E-anti, 10Z-sym, 1

biliverdins. IT 130877-88-2

RL: RCT (Reactant); RACT (Reactant or reagent)

(hydrolysis of) RN 130877-88-2 CAPLUS

80 130e7/-06-Z UEF005 CM Pyrrolo[1,2-a] pyrrolo[1111,2111,7111] axepino[411,5111,511] pyrrolo[1,111,511] axepino[411,5111,511] pyrrolo[2,3-d] axepino[41,511] axepino[41,51

PAGE 1-B

- OMe

II 130877-84-8P 130888-62-9P
RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation and reduction by chemical reagent or mammalian biliverdin reductase.

structure relation to)

RN 130877-84-8 CAPLUS

CN Pyrrolo[1,2-a pyrrolo[1",2"":1",7""] azepino[4",5"",5"] pyrrolo[1",2":1",7"] azepino[4",5",5"] pyrrolo[1",2":1",7"] azepino[4",5",4",5"] pyrrolo[2,3-d] azepino[4",5",4",5"] pyrrolo[2,3-d] azepino[4",5",5",6",5"] pyrrolo[2,3-d] azepino[4",5"] pyrrolo[2,3-d] azepino[4",5"] pyrrolo[4",5"] pyrrolo[4",5"

RN 130888-62-9 CAPLUS

CN Dipyrrolo[1,2-a:2',3'-d]azepine-8-propanoic acid, 2-[[8-(2-carboxyethyl)-4,5-dihydro-3,9-dimethyl-7-oxodipyrrolo[1,2-a:2',3'-dlazepin-2(7H)-ylidene|methyl-1-4,5',7-teterahydro-3,9-dimethyl-7-oxo-,

(Z)- (9CI) (CA INDEX NAME)
Double bond geometry as shown.

PAGE 1-B

_ CO2H

IT 130877-89-3P 130877-90-6P

RL: SPN (Synthetic preparation); PREF (Preparation) (preparation of, extended or helical conformation effects on mercapto group nucleophilic addition in)

RN 130877-89-3 CAFLUS
CN Pyrrolo[1,2-a]pyrrolo[1",2":1",7"]azepino[4",5":4",5"]pyrrolo[1,2-a]pyrolo[1,2-a]pyrolo[2,3-d]azepino-2,12-dipropanolo acid, 3,5,6,7,8,13,15,16-octahydro-18-[(2-hydroxyethyl)thio]-1,11,17-trinethyl-3,13-dioxo (CA INDEX NAME)

RN 130877-90-6 CAPLUS

CN Dipyrrolo[1,2-a:2',3'-d]azepine-8-propanoic acid, 2-[18-(2-arrboyspity)]-1,4,5,7-tetralpyro-3,9-dinethyl-7-oxodipyrrolo[1,2-a:2',3'-d]azepin-2-yl][(2-hydroxyethyl)thio]nethylene]-2,4,5,7-tetralpydro-3,9-dinethyl-7-oxo-(2)-(9CI) [CR INEES INME]

IT 130888-64-1

CN

RL: RCT (Reactant); RACT (Reactant or reagent) (saponification of)

RN 130888-64-1 CAPLUS

Dipyrrolo[1,2-a:2',3'-d]azepine-8-propanoic acid,
2-[14,5-dhydro-8-(3-methoy-3-oxopropyl)-3,9-dimethyl-7-oxodipyrrolo[1,2-a:2',3'-d]azepin-2(7B)-ylidene]methyl]-1,4,5,7-tetrahydro-3,9-dimethyl-7-oxo-, methyl ester, (2)- (SCI) (CAINDEX NAME)

Double bond geometry as shown.

PAGE 1-B

, ome

OS.CITING REF COUNT: 5 THERE ARE 5 CAPLUS RECORDS THAT CITE THIS RECORD (5 CITINGS)

L29 ANSWER 21 OF 27 CAPLUS COPYRIGHT 2011 ACS on STN

ACCESSION NUMBER: 1989:75127 CAPLUS DOCUMENT NUMBER: 110:75127

ORIGINAL REFERENCE NO.: 110:12401a,12404a TITLE: Total synthesis of "extended" biliverdins. The

relation between their conformation and their spectroscopic properties AUTHOR (S): Iturraspe, Jose B.; Bari, Sara; Frydman, Benjamin

CORPORATE SOURCE: Fac. Farm. Bioquim., Univ. Buenos Aires, Buenos Aires, 1113, Argent.

Journal of the American Chemical Society (1989),

111(4), 1525-7 CODEN: JACSAT: ISSN: 0002-7863

DOCUMENT TYPE: Journal. LANGUAGE: English

Extended biliverdins of the neopterobilin type, e.g., I, were obtained by treatment of Z,Z,Z-2-chloroethylbiliverdins, e.g., II, with DBU at 25°. When the 2-chloroethyl residue was at C(7), rotation at the C(5)-C(6) bond allowed a 52-syn to 52-anti conformational change followed by an intramol. alkylation at N(21). A seven-membered ring was thus formed, which kept the new biliverdin in a 52-anti, 102-syn 152-syn conformation. When two 2-chloroethyl residues at C(7) and C(13) were present in the bilitriene, the DBU treatment afforded a 5Z-anti, 10Z-syn, 152-anti biliverdin with two seven-membered rings which resulted from the intramol, alkylation at N(21) and N(24). When the 2-chloroethyl chain was

AB

at C(8), a seven-membered ring was formed by alkylation at N(23) and the resulting biliverdin had a 58-syn, 108-anti, 158-syn conformation. The HI-MMR spectra of the extended biliverdins are concentration dependent, indicating that these biliverdins (unlike those with a helicoida)

conformation) associate in solution. Their spectra were also temperature dependent and

at -80 °C a mixture of conformers could be detected. The s

vin/s UV ratio of the extended bilivordins increased about a 40-fold over the ratio of the helical-shaped bilivordins, a fact that can be useful for the interpretation of the spectra of biliproteins. 118631-57-59 18631-58-69 118631-60-0P

IT 118631-57-5P 118631-58-6P 118631-60-0P RL; SPN (Synthetic preparation); PREP (Preparation)

(preparation, conformation, and spectral characterization of)

CN IH-Pyrrole-3-propancic acid, 2-[[2-[6-ethenyi-1, 4, 5, 7-tetrahydro-3, 9-disethyl-7-roxed]pyrrolo[1,2-a:2], 3-d|azepln-2-y]laethylene[4-4]-sethoxy-3-oxopropy], 3-sethyl-2H-pyrrol-5-y]laethylene[-2, 5-dihydro-4-methyl-5-oxopentyl-2H-pyrrol-5-y]laethylene[-2, 5-dihydro-4-methyl-5-oxopentyl-2H-pyrrol-5-y]

Double bond geometry as shown.

RN 118631-58-6 CAPLUS

CN Dipytrolo[1,2-a;2',3'-d]azepine-9-propanoic acid, 2-[14,5-dihydro-9',3-methowy-3-oxopropyl-3,8-dimethyl-7-oxodipytrolo[1,2-a;2',3'-d]azepin-2(7ll)-ylidene]methyl]-1,4,5,7-tetrahydro-3,8-dimethyl-7-oxo-, sethyl ester, (2)- (SCI) [CAINDEX MME]

Double bond geometry as shown.

RN 118631-60-0 CAPLUS

GR 11E-Pyrrole-3-propanoic acid, 2-[12-1(6-ethenyl-1.4,5,7-tetrahydro-3,9-disethyl-7-roxodisprotolol_2-acid,2-(3-disethyl-2-yl-6-fiss)) methylene|-4-(3-methoxy-3-oxopropyl)-3-methyl-2-fis-pyrol-5-yl-]methylene|-2,5-dihydro-4-methyl-5-oxo-, methyl ester, (K, 2,7-(9CI) (CA INEX NAME))

Double bond geometry as shown.

OS.CITING REF COUNT: 6 THERE ARE 6 CAPLUS RECORDS THAT CITE THIS RECORD (6 CITINGS)

L29 ANSWER 22 OF 27 CAPLUS COPYRIGHT 2011 ACS on STN

LZ9 ANSWER ZZ OF Z/ CAPLUS COPINIGHT ZUII ACCESSION NUMBER: 1985:578184 CAPLUS DOCUMENT NUMBER: 103:178184

ORIGINAL REFERENCE NO.: 103:28675a,28678a
TITLE: Firm evidence for cis-aminopalladation in the reaction

of 1-aminohexatrienes with palladium dichloride
AUTHOR(S): Isomura, Kazuaki; Okada, Norivuki; Saruwatari, Masumi;

Yamasaki, Hirotaka; Taniguchi, Hiroshi
Fac. Eng., Kyushu Univ., Fukuoka, 812, Japan
SOURCE: Chemistry Letters (1985), (3), 385-8

CODEN: CMLTAG; ISSN: 0366-7022

DOCUMENT TYPE: Journal LANGUAGE: English

OTHER SOURCE(S): CASREACT 103:178184

AB The reaction of PGC12(PRCN)2 with Et --acetamico-P-(4,6-dimethylbenozofuran-2-yl)acrylate I having a 2-propenyl group at 2-position of benzofuran ring, gave an azepine derivative II, whoreas its E-isomor afforded a Pd-o-complex having azepine skeleton III. Configurational assignment of the e-complex,

accomplished by methoxycarbonylation, clearly demonstrates that this intramol. aminopalladationproceeds via cis-aminopalladation.

98796-41-9P 98796-42-0P 98796-43-1P RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of) RN 98796-41-9 CAPLUS

RN 98796-41-9 CAPLUS CN 1H-Benzofuro[2,3-d]azepine-4-carboxylic acid,

3-acetyl-2,3-dihydro-2,8,10-trimethyl-, ethyl ester (CA INDEX NAME)

RN 98796-42-0 CAPLUS

1H-Benzofuro[2,3-d]szepine-1,4-dicarboxylic acid, 3-acetyl-2,3-dihydro-2,8,10-trimethyl-, 4-ethyl 1-methyl ester, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 98796-43-1 CAPLUS CN 1H-Benzofuro[2,3-d

1H-Benzofuro[2,3-d]azepine-1,4-dicatboxylic acid,
3-acetyl-2,3-dihydro-2,8,10-trimethyl-, 4-ethyl 1-methyl ester, trans(SCI) (CA INDEX NAME)

Relative stereochemistry.

IT 98796-40-8P

RL: RCT (Reactant); SFN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation, hydrogenation, and methoxycarbonylation of)

RN 98796-40-8 CAPLUS

CN Palladium, [3-acetyl-4-(ethoxycarbonyl)-2,3-dihydro-2,8,10-trimethyl-1H-

benzofuro[2,3-d]azepin-l-yl]chloro-, cis- (9CI) (CA INDEX NAME) Relative stereochemistry.

OS.CITING REF COUNT: 9 THERE ARE 9 CAPLUS RECORDS THAT CITE THIS RECORD (9 CITINGS)

L29 ANSWER 23 OF 27 CAPLUS COPYRIGHT 2011 ACS on STN

ACCESSION NUMBER: 1981:460867 CAPLUS

DOCUMENT NUMBER: 95:60867 ORIGINAL REFERENCE NO.: 95:10283a,10286a

TITLE: Palladium-promoted formation of azepines from

1-aminohexatrienyl system

AUTHOR(S): Hatano, Sumiko; Saruwatari, Masumi; Isomura, Kazuaki; Taniguchi, Hiroshi

CORPORATE SOURCE: Fac. Eng., Kyushu Univ., Fukuoka, 812, Japan SOURCE: Heterocycles (1981), 15(2), 747-52

CODEN: HTCYAM; ISSN: 0385-5414 DOCUMENT TYPE: Journal

DOCUMENT TYPE: Journal LANGUAGE: English OTHER SOURCE(S): CASREACT 95:60867

AB Treatment of Et α-amino-β-(3-alkenylbenzofuran-2-yl)acrylate

(the 1-aminohexatrieny; system) with PGC12 (PBCN)2 in the presence of NaZCO3 qave azepines via a selective cyclization of the NH2 group to the terminal cation of the alkenyl group in an intramol. aminopalladation. The mechanism of this reaction and the acid catalyzed formation of Et

dibenzofurancarboxylates was discussed.
T 78347-79-2P 78347-82-7P 78347-83-8P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 78347-79-2 CAPLUS CN 1H-Benzofuro[2,3-d]az

1H-Benzofuro[2,3-d]azepine-4-carboxylic acid.

2,3-dihydro-8,10-dimethyl-1-methylene-, ethyl ester (CA INDEX NAME)

RN 78347-82-7 CAPLUS

CN 1H-Benzofuro[2,3-d]azepine-4-carboxylic acid, 3-acetyl-2,3-dihydro-8,10-dimethyl-, ethyl ester (CA INDEX NAME)

RN 78347-83-8 CAPLUS

N 1H-Benzofuro[2,3-d]azepine-4-carboxylic acid, 3-acetyl-2,3-dihydro-, ethyl ester (CA INDEX NAME)

OS.CITING REF COUNT:

1

THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD (1 CITINGS)

L29 ANSWER 24 OF 27 CAPLUS COPYRIGHT 2011 ACS on STN

ACCESSION NUMBER: 1980:495115 CAPLUS DOCUMENT NUMBER: 93:95115

ORIGINAL REFERENCE NO.: 93:15245a,15248a

TITLE: Synthesis of pyrroles, pyridines, and azepines from 2H-azirines AUTHOR(S): Saruwatari, Masumi; Hatano, Sumiko; Isomura, Kazuaki;

Taniguchi, Hiroshi CORPORATE SOURCE: Fac. Eng., Kyushu Univ., Fukuoka, Japan

Fukusokan Kagaku Toronkai Koen Yoshishu, 12th (1979), 211-15. Kitasato Daigaku Yakugakubu: Tokyo, Japan.

CODEN: 42VC39 DOCUMENT TYPE: Conference Japanese

LANGUAGE:

The controlling factor for the formation of pyrroles, pyridines, and AB azepines (e.g. I-III) from 2H-azirines (e.g. IV, R - H, Me, Ph) were discussed with mechanistic detail.

63325-41-7P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)

RN 63325-41-7 CAPLUS

CN 5H-Benzofuro[2,3-d][1]benzazepine-6-carboxylic acid, ethyl ester (CA INDEX NAME)

L29 ANSWER 25 OF 27 CAPLUS COPYRIGHT 2011 ACS on STN

ACCESSION NUMBER: 1978:152465 CAPLUS DOCUMENT NUMBER: 88:152465

ORIGINAL REFERENCE NO.: 88:24025a,24028a

TITLE: Studies on heterocyclic compounds, XLIII, Reaction of 1-phenyl-4-hydrazino-4,5-dihydro-6H-furo(2,3dl[1]benzazepine-5-carboxylic acid hydrazide with

aromatic aldehydes AUTHOR (S): Ito, Kazuo; Yakushijin, Kenichi; Yoshina, Shigetaka CORPORATE SOURCE:

Fac. Pharm., Meijo Univ., Nagoya, Japan SOURCE . Heterocycles (1978), 9(2), 169-73

CODEN: HTCYAM; ISSN: 0385-5414 DOCUMENT TYPE: Journal English

LANGUAGE:



The title compound (I; R - H) reacted with RICHO (R1 - 2-furyl, Ph, AB

p-C1C6H4) in EtOH to give I (R2 = CHR1) and the monoarylidene derivative II. 66206-57-3P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation and condensation with aldehydes)

66206-57-3 CAPLUS RN

6H-Furo[2,3-d][1]benzazepine-5-carboxylic acid, 1-phenyl-, hydrazide (CA CN INDEX NAME)

IT 63874-16-8P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and reaction with hydrazine)

RN 63874-16-8 CAPLUS

6H-Puro[2,3-d][1]benzazepine-5-carboxylic acid, 1-phenyl-, ethyl ester CN

(CA INDEX NAME)

IT 66206-53-9P 66206-54-0P 66206-55-1P RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of)

RN 66206-53-9 CAPLUS CN 6H-Puro[2,3-d][][benzazepine-5-carboxylic acid, 1-phenyl-, 2-(2-furanylmethylene)hydrazide (CA INDEX NAME)

RN 66206-54-0 CAPLUS

CN 6H-Furo[2,3-d][1]benzazepine-5-carboxylic acid, 1-phenyl-, 2-(phenylmethylene)hydrazide (CA INDEX NAME)

RN CN

66206-55-1 CAPLUS 6H-Furo[2,3-d][1]benzazepine-5-carboxylic acid, 1-phenyl-, 2-[(4-chlorophenyl)methylene]hydrazide (CA INDEX NAME)

L29 ANSWER 26 OF 27 CAPLUS COPYRIGHT 2011 ACS on STN

LZ9 ANSWER Z6 OF Z/ CAPLUS COPIRIGHT ZUI1 ACCESSION NUMBER: 1977:502204 CAPLUS DOCUMENT NUMBER: 87:102204

ORIGINAL REFERENCE NO.: 87:16223a,16226a
TITLE: Studies on heterocyclic compounds. Part XXXI.

Synthesis of ethyl 1-phenyl- and

2-methyl-6H-furo[2,3-d][1]benzazepine-5-carboxylates
AUTHOR(S): Yakushijin, Kenichi; Yoshina, Shigetaka; Tanaka, Akira

CORPORATE SOURCE: Fac. Pharm., Meijo Univ., Nagoya, Japan SOURCE: Heterocycles (1977), 6(6), 721-5

CODEN: HYCYAM; ISSN: 0385-5414

DOCUMENT TYPE: Journal LANGUAGE: English

LANGUAGE: English
OTHER SOURCE(S): CASREACT 87:102204

AB Thermolysis of I (R - Fh, R1 - H; R - H, R1 - Me) in ligroin gave II, which on thermolysis in boiling sylene gave III. Reduction of III with Zn in AcOH gave IV (R2 = COZEI), which when treated with NABBH in EXOH gave IV (R2 = CIXOH), which was also obtained by direct reduction of III with NABBH in EXOH gave IV

IT 63874-16-8P 63874-17-9P RI: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and reduction of) 63874-16-8 CAPLUS

RN 63874-16-8 CAPLUS CN 6H-Furo[2,3-d][1]benzazepine-5-carboxylic acid, 1-phenyl-, ethyl ester (CA INDEX NAME)

RN 63874-17-9 CAPLUS CN 6H-Furo[2,3-d][1]benzazepine-5-carboxylic acid, 2-methyl-, ethyl ester (CA INDEX NAME)

L29 ANSWER 27 OF 27 CAPLUS COPYRIGHT 2011 ACS on STN

ACCESSION NUMBER: 1977:453010 CAPLUS DOCUMENT NUMBER: 87:53010

ORIGINAL REFERENCE NO.:

TITLE: Compelled azepine ring formation in thermal ring expansion of 2H-azirine

AUTHOR(S): Isomura, Kazuaki; Taguchi, Hiroshi; Tanaka, Tatsuyoshi; Taniguchi, Hiroshi

CORPORATE SOURCE: Fac. Eng., Kyushu Univ., Fukuoka, Japan SOURCE: Chemistry Letters (1977), (4), 401-4

CODEN: CMLTAG; ISSN: 0366-7022 DOCUMENT TYPE . Journal. English

LANGUAGE:

AB Thermolyses of benzofuran-2-ylvinyl azides I (R = H, Me, Ph) gave benzofuropyrrole II, benzofuropyridine III, and benzofurobenzazepine IV, resp. Photolysis of these azides gave the corresponding 2H-azirines V, which on heating gave the same heterocyclic comdps., II-IV, as arose from the thermolysis of I.

63325-41-7P RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of) RN 63325-41-7 CAPLUS

CN 5H-Benzofuro[2,3-d][1]benzazepine-6-carboxvlic acid, ethyl ester (CA INDEX NAME)

OS.CITING REF COUNT: 3 THERE ARE 3 CAPLUS RECORDS THAT CITE THIS RECORD (3 CITINGS)